STUDIES OF RADIOACTIVE COMPOUNDS:
I—VANDENBRANDEITE[1]

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ABSTRACT

Vandenbrandeite is triclinic with a 7.84, b 5.43, c 6.09 kX; α 91°52', β 102°00', γ 89°37' and cell content $2[CuUO_4 \cdot 2H_2O]$. An angle table has been calculated and powder data are given.

The usual method of defining crystal systems in terms of crystallographic axes is inadequate; the classification of crystals must rest on the symmetry that has its origin in the atomic arrangements. A review of rules for orienting triclinic crystals suggests that the one important standardization is in the selection of the conventional structural cell, which has as edges the three shortest noncoplanar translations in the lattice. This cell is easily recognized from its dimensions and angles regardless of the setting, and is readily reoriented for a special purpose. The preferred orientation of the cell should if possible, have α and β obtuse, and $a < b$. It should be designed to best describe the mineral. Any noteworthy property, such as structural or morphological analogy to other minerals should influence the choice of setting; in the absence of an outstanding feature morphological crystallographers will probably continue to designate some prominent direction within the crystal as the c axis.

Vandenbrandeite is a hydrous copper uranate which has been found only in the Katanga district of the Belgian Congo. The mineral was first described and named by Schoep (1932), who studied material from Kalongwe. Thoreau (1933) later reported it from Shinkolobwe under the name uranolepidite. The published observations of these two men leave little doubt of the identity of vandenbrandeite and uranolepidite. We are indebted to them for two chemical analyses and a description of the physical and optical properties that is adequate for future identification of the mineral. However, the crystallography of vandenbrandeite has not been fully studied. Crystal measurements leading to axial ratios have not been made and the triclinic symmetry has been inferred on the basis of optical examinations. Hence the mineral offered an interesting and useful study.

Through the kindness of Professor V. B. Meen, we were fortunate to obtain the loan of a specimen (ROM M18598) from the type locality of Kalongwe which had been presented to the Royal Ontario Museum of Geology and Mineralogy by M. Thoreau. This specimen is composed of massive dark green vandenbrandeite containing minute (to $\frac{1}{3}$ mm.)

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tabular crystals of the mineral in vugs. The crystals are partially covered by a light brown deposit which was identified as kasolite with an x-ray powder photograph.

The optical properties proved most useful in establishing the identity of our material with that studied by Schoep and Thoreau. Under the polarizing microscope fragments of the mineral show moderate pleochroism with colours varying from yellow-green to blue-green. Fragments lying on the excellent cleavage are blue-green in colour, not pleochroic and have a very low birefringence. They are within 5° of being perpendicular to an optic axis and it is therefore possible to make a fairly accurate determination of the Y index. The optical data we obtained are compared below with those of Schoep and Thoreau:

	Schoep	Thoreau	Milne and Nuffield
X	1.77 ± 0.02	1.76	1.765 ± 0.005
Y	1.78 ± 0.02	—	1.792 ± 0.002
Z	1.80 ± 0.02	1.80	—
$2V$	—	large	near 90°

Thoreau gave the optical sign as negative but Schoep's indices of refraction require a positive sign. Optical measurements on our material were made difficult by a great number of inclusions. Schoep considered these to be kasolite and this is supported by the presence of this mineral on the crystal faces of vandenbrandeite. In addition to solid inclusions, many rounded liquid inclusions containing gas bubbles were seen.

The cleavage referred to above is parallel to (110) in our setting and is the only one we observed. The optical study indicates that this is the (001) cleavage of Schoep, who recorded a second direction and suggested the possibility of a third. Thoreau also observed three cleavages which he said caused the mineral to break into laths. It is possible that Schoep and Thoreau had better material than we did but we believe that the presence of the two additional cleavages should be accepted with reservations.

A study of the crystals showed that the tabular faces are characteristically rounded and poorly reflecting. However, some crystals have a zone of several well developed faces, the axis of which is inclined at about 13° to the normal of the tabular face. On the chosen crystal this axis, which was later designated as $c[001]$ was utilized as the rotation axis to obtain two-circle goniometric measurements of the faces, as well as rotation, and zero and first layer Weissenberg x-ray photographs. Consideration of the gnomonic and reciprocal lattice projections revealed triclinic symmetry and indicated that the rotation axis is one of the three shortest lattice translations. It was now possible to select the remaining two translations in the lattice and to locate their direction in

the crystal. To assure more accurate cell constants zero layer Weissenberg photographs were prepared by turning the crystal about these two directions. Measurement of the films gave $d(100)$ 7.67, $d(010)$ 5.43, $d(001)$ 5.95kX;[1] $\alpha*88°10'$, $\beta*78°00'$, $\gamma*90°00'$. From these values the reciprocal and direct cell elements were calculated:

Reciprocal cell		Direct cell	
$a*=0.1304$	$\alpha*=88°10'$	$a=7.84$ kX	$\alpha=91°52'$
$b*=0.1842$	$\beta*=78\ 00$	$b=5.43$	$\beta=102\ 00$
$c*=0.1681$	$\gamma*=90\ 00$	$c=6.09$	$\gamma=89\ 37$

The morphology of the crystal gives no reason to suspect the absence of a symmetry center. Therefore the mineral has been placed in space-group $P\bar{1}$. The usual x-ray powder data obtained on a clean sample is presented in Table 1, and the photograph itself is reproduced in Fig. 1.

FIG. 1. Vandenbrandeite: X-ray powder print; Cu/Ni; 1 mm.$=1°\vartheta$.

TABLE 1. VANDENBRANDEITE: X-RAY POWDER DATA

Triclinic-$P\bar{1}$; a 7.84, b 5.43, c 6.09; α 91°52', β 102°00', γ 89°37'

I	d(meas.)	I	d(meas.)	I	d(meas.)	I	d(meas.)
4	5.05 kX	2	1.963	$\frac{1}{2}$	1.417	$\frac{1}{2}$	1.066
10	4.28	1	1.909	$\frac{1}{2}$	1.395	$\frac{1}{2}$	1.053
2	3.84	3	1.847	2	1.345	$\frac{1}{2}$	1.042
2	3.71	$\frac{1}{2}$	1.819	$\frac{1}{2}$	1.330	$\frac{1}{2}$	1.035
2	3.32	1	1.789	3	1.314	$\frac{1}{2}$	1.026
1	3.06	$\frac{1}{2}$	1.747	$\frac{1}{2}$	1.297	$\frac{1}{2}$	1.018
8	2.91	1	1.705	$\frac{1}{2}$	1.273	$\frac{1}{2}$	1.010
$\frac{1}{2}$	2.76	$\frac{1}{2}$	1.682	2	1.250	$\frac{1}{2}$	1.001
4	2.55	$\frac{1}{2}$	1.654	$\frac{1}{2}$	1.243	1	0.988
$\frac{1}{2}$	2.47	2	1.621	1	1.224	$\frac{1}{2}$	0.976
$\frac{1}{2}$	2.39	$\frac{1}{2}$	1.576	$\frac{1}{2}$	1.195	$\frac{1}{2}$	0.966
1	2.35	1	1.554	$\frac{1}{2}$	1.171	1	0.952
1	2.28	1	1.524	$\frac{1}{2}$	1.154	1	0.942
$\frac{1}{2}$	2.19	1	1.495	$\frac{1}{2}$	1.127	1	0.937
$\frac{1}{2}$	2.15	3	1.469	2	1.094	1	0.929
3	2.09	$\frac{1}{2}$	1.435	2	1.074	$\frac{1}{2}$	0.925

[1] Using CuKα=1.5374 kX.

The choice of the setting of vandenbrandeite has been influenced by the close approach to monoclinic lattice geometry and by the tabular habit. The axis which is very nearly perpendicular to the other two was chosen as the b axis. Next the a axis was selected from the remaining two possibilities in order to describe the broad face as (001). Finally the positive directions of the axes were so chosen as to make α and β obtuse.

In this setting the crystals are tabular parallel to $c(001)$ and somewhat elongated parallel to the edge $c(001) \wedge m(110)$. The habit is portrayed in Fig. 2. The relative dimensions of the faces have been preserved as far as possible in the drawing, but the crystal has been idealized by the addition of the assumed center of symmetry. The crystals are commonly attached by $m(110)$ and grow outward in a direction defined by the edge $c(001) \wedge M(1\bar{1}0)$. Examination of the crystals gives one the impression that the mineral would exhibit a lozenge-shaped habit controlled by $m(110)$ and $M(1\bar{1}0)$ under conditions permitting greater freedom of crystal growth thus heightening the illusion of monoclinic symmetry.
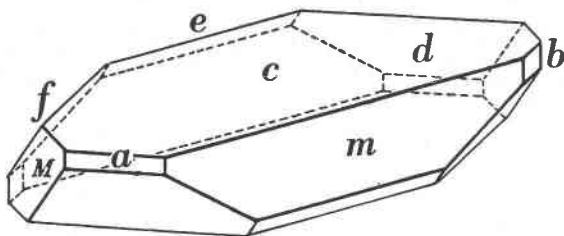

Fig. 2. Vandenbrandeite: crystal from Kalongwe, Katanga.

Crystals are so implanted on the massive material as to show $m(110)$, which is the excellent cleavage, to advantage. This probably influenced Schoep (1932) to describe it as $c(001)$. The crystal sketch which accompanies his description shows four other forms to three of which he assigned indices without deriving axial ratios from crystal measurements. It is possible to identify all the forms as follows:

Schoep	Structural
(001)	$m(110)$
(1$\bar{1}$0)	$c(001)$
(100)	$a(100)$
(110)	$d(10\bar{1})$
not named	$M(1\bar{1}0)$

The crystal faces are far from perfect and as a result, measurements on the two-circle goniometer proved inconsistent. On the other hand the rotation and zero-layer Weissenberg photographs about the three axial directions were sharp and yielded good results. Consequently the

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cell constants were used to calculate axial ratios and reciprocal and pro-jection elements and finally the angle table for the observed forms (Table 2). As a check on our calculations Table 3 has been prepared giving a comparison between the measured and calculated two-circle angles, ϕ and ρ for all the faces on the crystal. It is to be noted that the agreement between corresponding angles is usually within one degree and that there is no doubt that correct Miller indices have been as-signed to the faces.

TABLE 2. VANDENBRANDEITE: $CuUO_4 \cdot 2H_2O$

Triclinic, $P\bar{1}$

$a:b:c = 1.443:1:1.120$; $\alpha = 91°52'$, $\beta = 102°00'$, $\gamma = 89°37'$
$p_0:q_0:r_0 = 0.776:1.096:1$; $\alpha^* = 88°10'$, $\beta^* = 78°00'$, $\gamma^* = 90°00'$
$p_0' = 0.794$, $q_0' = 1.121$, $x_0' = 0.2127$, $y_0' = 0.0327$

Form	ϕ	ρ	A	B	C
$c(001)$	81°15′	12°09′	78°00′	88°10′	0°00′
$b(010)$	180 00	90 00	90 00	180 00	88 10
$a(100)$	90 00	90 00	180 00	90 00	78 00
$m(110)$	35 18	90 00	54 42	35 18	81 35
$M(1\bar{1}0)$	144 42	90 00	54 42	144 42	84 36
$f(0\bar{1}1)$	168 57	47 57	81 49	136 47	48 38
$d(\bar{1}01)$	−86 47	30 11	120 08	88 23	42 08
$e(\bar{1}\bar{1}2)$	−160 46	29 12	99 15	117 26	36 22

TABLE 3. VANDENBRANDEITE

Face	Measured		Calculated	
	ϕ	ρ	ϕ	ρ
$c(001)$	82°29′	12°25′	81°15′	12°09′
$\bar{b}(0\bar{1}0)$	180 00	90 00	180 00	90 00
$a(100)$	−87 51	90 00	−90 00	90 00
$m(110)$	35 20	89 43	35 18	90 00
$\bar{m}(\bar{1}\bar{1}0)$	−145 39	90 00	−144 42	90 00
$M(1\bar{1}0)$	144 36	90 00	144 42	90 00
$\bar{M}(\bar{1}10)$	−35 35	90 00	−35 18	90 00
$f(0\bar{1}1)$	168 54	46 55	168 57	47 57
$d(\bar{1}01)$	−87 56	29 12	−86 47	30 11
$e(\bar{1}\bar{1}2)$	−161 42	30 00	−160 46	29 12

Vandenbrandeite and the Bravais Rule

The "Law" of Bravais states that the importance (size and frequency) of crystal forms is proportional to reticular densities, or the spacings, of

the corresponding lattice planes; this implies that the rate of growth is proportional to lattice row density. Donnay and Harker (1937) extended this rule to include the effects of space group symmetry operations involving translation on the lattice spacings. The rules coincide for triclinic space groups since screw axes and glide planes are not involved. Mineral examples (Nuffield & Peacock, 1945) have been presented which support with certain exceptions, the Bravais rule in its modified form. Vandenbrandeite is the case of a mineral that differs remarkably from the ideal Bravais crystal.

To test the observed importance of crystal forms on vandenbrandeite against the theoretical importance demanded by the Bravais rule, Table 4 has been prepared. This table gives all the calculated spacings

TABLE 4. VANDENBRANDEITE: CALCULATED SPACINGS

α^* 88°10', β^* 78 00, γ^* 90 00

a 7.84, b 5.43, c 6.09kX; α 91°52', β 102 00, γ 89 37

Plane	d_{kX}	Form	Plane	d_{kX}	Form
(100)	7.67	a —small	($\bar{1}$11)	3.74	—
(001)	5.95	c —broad, dominant	($\bar{2}$01)	3.58	—
(010)	5.43	b —very small	(1$\bar{1}$1)	3.39	—
(10$\bar{1}$)	5.31	d —large	(111)	3.32	—
(1$\bar{1}$0)	4.43	M—large, smaller than m	(210)	3.13	—
(110)	4.43	m —second largest face	($\bar{2}$11)	3.02	—
(101)	4.26	—	($\bar{1}$02)	2.99	—
(01$\bar{1}$)	4.08	f —medium	(201)	2.96	—
(011)	3.95	—	(102)	2.69	—
($\bar{1}\bar{1}$1)	3.85	—	($\bar{1}\bar{1}$2)	2.66	e—small

in decreasing order to include the observed forms. The Bravais rule predicts that the three most important forms shall be (100), (001) and (010), decreasing in that order. The habit should be tabular parallel (100) with elongation if any parallel to b[010]. Actually (100) and (010) are among the smallest faces; crystals are tabular parallel to (001) and elongated parallel to the edge (001)$\wedge$(110) which is not an edge of the conventional cell. The appearance of the form ($\bar{1}$12) is another anomaly. It seems that the only point in support of the Bravais rule is the fact that 7 of the 8 observed forms are among the 8 largest spacings.

The lozenge-shaped crystal outline of vandenbrandeite is reminiscent of the habit displayed by certain base-centred monoclinic minerals like plagionite and semseyite (Nuffield & Peacock, 1945). The crystal outlines of these two minerals are due to the predominant development of the (hhl) and $(\bar{h}hl)$ zones and are in accord with the modified rule of

Bravais. The extinction condition characteristic of base-centring, (hkl) present only with $h+k$ even, halves the effective lattice spacings of (100) and (010) and consequently increases the relative theoretical importance of (hhl) and ($\bar{h}hl$) forms. Vandenbrandeite is analogous in that the crystallographic elements are pseudo-monoclinic; furthermore, two forms in the (hhl) and ($h\bar{h}l$) zones, m(110) and M(1$\bar{1}$0) dominate and largely determine the crystal outline. However, the Weissenberg photographs do not indicate a centred conditioned in the lattice. Consequently we are left with the interesting speculation that the structure falls just short of a base-centred condition, but nevertheless may influence crystal growth as though this condition were realized. However, many anomalies remain, in particular the absence of the 4 unit (hkl) pinakoids.

Despite the case just cited, a sufficient number of mineral examples are to be found in the literature to indicate that form development is often in accordance with the Bravais rule; many exceptions to this rule can be explained by the Donnay-Harker modification. It would however, be too much to expect crystal growth to proceed in all or even in most cases according to a rule based on purely geometrical considerations and which " . . . does not involve any consideration of the special positions that the atoms may occupy, nor does it take into account their nature, their charge, their bonds, or any other physical concept" (Donnay & Harker, 1937, p. 455). Buerger (1947) has pointed out that the characteristics of the particles which arrive at the crystal surfaces during growth are a fundamental factor in determining crystal habit. It would seem therefore, that these rules are but first approximations in the attempt to evaluate the influence of the atomic structure upon its form development. Instances of good agreement between crystal habit and the Bravais-Donnay-Harker rule suggest that in these cases the effects of the packing and bonding of atoms and of the environment of the crystal may be equated to the lattice in terms of the modified rule of Bravais. It appears that a study of the atomic structures of non-conforming crystals is necessary to broaden the scope of the rules.

Composition and Cell Content

Vandenbrandeite has been analyzed by Schoep (1932), and Boubnoff (in Thoreau, 1933). Both analyses (Table 5) indicate the presence of impurities and this is confirmed by the observation during this study of kasolite coating the crystal faces and of numerous inclusions within the crystals. Schoep adjusted his analysis by deducting PbO as kasolite ($3PbO \cdot 3UO_3 \cdot 3SiO_2 \cdot 4H_2O$) and by regarding Fe_2O_3 and P_2O_5 as impurities. In this paper Schoep's analysis has been adjusted by the withdrawal of PbO as kasolite on the basis of the now generally accepted formula for this mineral ($PbO \cdot UO_3 \cdot SiO_2 \cdot H_2O$). Each analysis with its

accompanying measured specific gravity has been used to calculate the cell contents. The results are given in Table 5. Clearly CuO and UO_3 approach 2. The values are below 2 probably because the measured specific gravities are too low, a logical deduction in view of the numerous liquid inclusions. The water content in both analyses is between 4 and 5 It is likely that the ideal value is 4 and the measured value is higher because of the abundance of liquid inclusions. The results point to the ideal cell content $2[CuO \cdot UO_3 \cdot 2H_2O]$ and this is the commonly accepted composition (Dana, 1944, p. 632). The calculated specific gravity is 5.26.

TABLE 5. VANDENBRANDEITE: ANALYSIS AND CELL CONTENTS
CELL VOLUME 253.5kX[3]

	I			II			III	
	A	B	C	A	B	C	A	B
CuO	15.78	18.77	1.87	18.98	19.20	1.91	19.81	2
UO_3	65.45	70.69	1.78	70.40	71.23	1.85	71.22	2
H_2O	9.25	10.54	4.41	9.46	9.55	4.08	8.97	4
PbO	4.69	—	—	—	—	—	—	—
SiO_2	1.66	—	—	0.28	—	—	—	—
Total	98.59[1]	100.00		99.95[2]	100.0		100.00	
G	4.96 (meas.)			5.03 (meas.)			5.26 (calc.)	

I. Kalongwe, Katanga district, Belgian Congo. A. Anal. Schoep (1932); [1]incl. Fe_2O. 1.55, P_2O_5 0.21. B. Analysis corrected by deducting kasolite ($PbO \cdot UO_3 \cdot SiO_2 \cdot H_2O$), SiO_2, Fe_2O_3 and P_2O_5 and summing to 100 per cent. C. Cell contents calculated for the cell volume and measured specific gravity 4.96.

II. Shinkolobwe, Katanga district, Belgian Congo. A. Anal. Boubnoff (in Thoreau, 1933); [2]incl. CaO 0.26, MgO 0.57. B. Analysis recalculated to 100 per cent after deducting SiO_2, CaO and MgO. C. Cell contents calculated for the cell volume and measured specific gravity 5.03.

III. A. Calculated weight per cent and specific gravity for $2[CuO_4 \cdot 2H_2O]$. B. Ideal cell contents.

THE CONVENTIONAL TRICLINIC CELL AND ITS SETTING

During the course of this study we had occasion to examine some of the literature concerned with the definition and description of a triclinic species. It became apparent that a summary and discussion of recent published works on the subject would be of value at the present time.

The Triclinic System

Crystal systems are usually defined in terms of the geometry of unit cells, or with reference to crystallographic axes by authors of textbooks.

The following abstracts illustrate this common practice. "Crystals lacking symmetry of any kind naturally have the most 'general' type of unit cell, the three axes of which are all inclined to each other at different angles and unequal in length. The addition of a centre of symmetry does not alter the situation . . . " (Bunn, 1945, p. 47). "In the triclinic system there are three crystallographic axes of unequal length that make oblique angles with each other" (Hurlbut, ed. 15, p. 57). "The triclinic system includes all crystals which are correctly referred to three unequal crystal axes intersecting each other at unequal angles. In general all three angles are oblique, but by chance one of them may be a right angle" (Winchell, 1942, pp. 106–107). "In the Triclinic System the crystallographic axes are all unequal and none is at right angles to another" (Rutley, 1936, p. 114). "The three axes in this system (Anorthic) being not only unequal in length, but also inclined to each other at different angles, none of which is a right angle . . . " (Miers, 1929, p. 87). It is not unusual to find that the crystal systems are distinguished on the basis of the geometry of space lattices. These expressions represent a peculiar anomaly in view of the fact that the systems are usually regarded as groups of crystal classes which in turn are almost universally regarded as symmetry combinations. Evidence will be presented in the following paragraphs to show that descriptions of systems based on the crystallographic axes are inadequate.

A crystal may be considered as a homogeneous structure consisting of an infinite number of identical units (unit cells) stacked in three dimensions; this implies that the structure may be attained by repeated and equal translations of the unit along its three edges.

Identical arbitrary points in the structure form a regular three-dimensional framework in space known as a point space lattice. The geometry of the crystal is in harmony with the geometry of this lattice. It follows that the crystallographic axes of the properly chosen morphological unit coincide in direction with the edges of the structural unit and with certain translation directions within the lattice. It can be readily appreciated that the crystallographic axes, the lattice and the cell edges are devices that define merely the geometry of the unit cell since they do not take full account of the symmetry of the atomic structure; therefore the symmetry of these geometrical devices need not be the same as the symmetry of the structure. The positions relative to one another of the identity points within the structure define the shape and therefore the symmetry of the lattice. This symmetry cannot be lower than that of the structure; in fact its symmetry is never lower than that of the highest symmetry class in the system of crystallization (or subsystem if hexagonal). Actually the identity points may outline a lattice that has higher symmetry than the structure; it is conceivable for a tri-

clinic crystal to have a lattice with cubic geometry and therefore cubic-like crystals referable to three equal axes inclined to each other at right angles. It becomes apparent that crystal systems cannot be accurately defined in terms of either the symmetry or the geometry of lattices, crystallographic axes or unit cells. The classification of crystals into systems and classes must rest on the symmetry of the atomic arrangements.

It is evident then that the above abstracted statements refer to specific cases. The general and therefore the more complete statement of a crystal system should give a description of its characteristic symmetry and the limitation this symmetry imposes on the generality of the geometry of unit cells, lattices or crystal axes. For example, triclinic minerals have only one-fold symmetry axes $(\bar{1}, 1)$; this symmetry imposes no restriction on the lengths of the 3 axes of the unit cell or their angular inclinations to one another.

The Conventional Triclinic Cell

There is general agreement among crystallographers that except in special cases, the properly chosen triclinic structural cell has as edges the three shortest noncoplanar translations in the lattice. In the geometrical sense there are two types of triclinic cells with oblique angles: those in which three obtuse interaxial angles may be chosen (Fig. 4) and those in which only two of the angles may be obtuse (Fig. 3), although three acute angles may be chosen. Donnay (1943) has pointed out that statements based on the assumption that it is always possible to select three obtuse interaxial angles have appeared in widely-used texts.

The selection of the morphological unit was formerly the cause of much thought and discussion among crystallographers and resulted in much attention being directed towards form development and crystal habit. Today the structural unit is the basis of almost all morphological descriptions and therefore the units are geometrically identical. Since the use of x-rays has become so common in mineralogy and the selection of the proper structural unit almost routine, the rules for selecting the morphological unit have lost much of their significance. However, studies of the form development of triclinic crystals have a practical application; frequently one of the edges of the conventional structural cell is parallel to the most prominent zone in a crystal or is roughly normal to the broad face of a tabular crystal. Peacock (1937a) has demonstrated that it is often possible to select the conventional structural unit from the gnomonic projection of a well-developed crystal if one of the cell edges can be located in the crystal. The problem is to recognize points of the first layer of the reciprocal lattice in the gnomonic projection of the known forms.

The unit cell is conventionally oriented so that the c axis is vertical and the a axis is directly fore and aft. This results in (010) being projected directly to the right in gnomonic and stereographic projections.

The Setting of Triclinic Crystals

The literature which deals with the setting of a triclinic crystal, that is with the designation of crystallographic axes and angles within the cell is far from clear-cut and is apt to be confusing to the casual crystallographer. It may be of value to briefly review some of the proposals and rules that have received much prominence.

Donnay, Tunell & Barth (1934) regarded the selection of the "main zone" (to be designated the c-axis) of first importance in the problem of selecting the proper morphological setting or orientation. This zone was taken as the direction of elongation (in prismatic or acicular crystals) or perpendicular to the plane of flattening (tabular habit). They suggested that the a axis slope forward and the b axis slope to the right (which is equivalent to α and β obtuse and implies that the base slopes forward and to the right of the projection of (100)) and that a be taken shorter than b. The authors pointed out that these rules although arbitrary, were actually the conventions practiced by most crystallographers.

Peacock (1937a) discussed the Donnay-Tunell-Barth morphological setting at some length and named it the normal setting. He extended the idea of the "main zone" to include the prominent edge of a habitually elongated crystal tabular to a plane in the elongated zone. In redefining the steps leading to this setting he limited the slope of the base to the front-right quadrant. This condition was defined alternately as $\phi001$ between $0°$ and $90°$, and α and β obtuse. Later (Peacock, 1937b) the inconsistent statement, α and β obtuse, was discarded, but still later (Donnay, 1943, p. 319) he returned to the original Donnay-Tunell-Barth rule: α and β obtuse.[1]

Buerger (1942) proposed rules leading to a unique setting which entirely disregard the morphology of crystals in favor of purely geometrical relationships within the structural cell. He advocated labelling the three shortest translations so that $a < b < c$ and choosing the positive ends of the axes so as to make α, β and γ all obtuse. These rules are applicable only to a cell of the type shown in Fig. 4 and are therefore, not of general use.

Donnay (1943) pointed out (as did Peacock, 1937a) that the "main zone" is often an edge of the conventional structural unit; in the case of minerals elongated parallel to this zone, the edge is frequently the short-

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[1] In Dana (1944, p. 6) the normal setting with the slope of the base to the front-right quadrant is favoured.

est lattice period. Since the direction of elongation in prismatic crystals is usually taken as the c axis in triclinic crystals, the arrangement $c < a < b$ has long been a common convention. Donnay further pointed out that the concept of the "main zone" lacked clarity; it had been defined as a zone of elongation, as the normal to a broad face, as a zone rich in faces, etc. Donnay therefore proposed to abandon the rule to set the axis of the "main zone" vertical in favour of designating the shortest axis c, but retained the conditions a less than b, and α and β obtuse. In effect Donnay has forged the most common conventions into an inflexible rule. Donnay recognized the recurrence of certain special problems (unusual habit, pseudosymmetry, etc.) which might make this rule unsatisfactory. He therefore agreed to relax his rule to the extent of permitting a cyclic permutation limited to three alternatives: (1) $c < a < b$, α and β obtuse; (2) $a < b < c$, β and γ obtuse; (3) $b < c < a$, γ and α obtuse.

The proposals which have been reviewed above are of two types: (1) those which emphasize a consideration of the crystal habit and form development (Donnay-Tunell-Barth, 1934; Peacock, 1937a) and (2) those based on geometrical considerations (Buerger, 1942; Donnay, 1943). It has already been pointed out that Donnay's rules are an attempt to compromise between these two extreme views.

An examination of triclinic settings published in the last 15 years shows that two customs, α and β obtuse, and $a < b$ continue to be much used whether the approach to the problem be from the morphological or the geometrical angle. These customs now have almost the status of rules.

No one convention, with respect to the length of c relative to a and b, is as clearly defined. The Donnay-Tunell-Barth convention regarding designation of the main zone as the c axis is still popular. It has already been mentioned that in the case of triclinic prismatic crystals this often results in the setting $c < a < b$. Contributing to its frequency is the fact that this setting is also selected at times without reference to crystal morphology. The setting $a < c < b$ is not uncommon and results from considerations which are morphological.

Practicing crystallographers frequently choose a setting for the purpose of emphasizing pseudosymmetry, morphological analogy, structural similarity, unusual crystal habit or form development, etc. The resulting crystallographic elements may deviate from the conventional.

Rules based on a consideration of the morphology of crystals cannot lead to a unique setting in all cases. The morphological approach is based on the concept that a mineral has a typical habit and that one of the edges of the conventional cell is parallel to the "main zone." It is probably true that most minerals have an average habit; if a sufficient number

of crystals from a variety of localities are examined, certain morphological characteristics will appear. It is probable that a unique setting could be attained for a majority of minerals if the characteristic crystal habit and form development were known. However, first descriptions of crystals are often based on a single specimen from one locality and the morphological development may be quite unusual. Furthermore, the concept of the "main zone" is often open to more than one interpretation on a crystal. For example, the authors first selected the $m \wedge c$ edge on vandenbrandeite as the "main zone" because crystals are elongated parallel to this edge and because it is the zone containing most of the large faces, one of which is the cleavage direction. Our next choice for the "main zone" was the "correct" one: a direction roughly normal to the broad face, containing again the cleavage, and smaller although perhaps some better-developed faces.

Rules that are geometrical have the advantage of leading to a unique setting if the unit is correctly determined by x-rays. However this advantage does not loom as large today. The problem of attaining the proper crystallographic elements was a matter of great concern to geometrical crystallographers of the past. Once the symmetry had been determined, this problem could be resolved into two parts: the selection of the morphological unit, and its orientation in some pleasing or useful way. The first task was the real crux of the problem. That no single straight-forward solution could be found is evident from the various principles and "laws" that were put forward for the guidance of crystallographers. This problem no longer exists for the majority of minerals. The need to find a unique setting from a study of crystal habit and form development is gone because the selection of the conventional structural cell (which is geometrically equivalent to the morphological unit) is now a routine matter with proper x-ray equipment and is controlled by accepted conventions. Today practically all morphological descriptions are based on and accompanied by x-ray data on the conventional unit cell. Although this cell may be oriented in 24 ways, its dimensions are always the same and its angles can differ only by becoming supplementary to those of another orientation. It is therefore easily recognized in contrast to the morphological unit in which the dimensions are given as axial ratios and not readily recognized in another orientation. Reorientation of the cell to another setting for the purpose of a general systematic treatment is a simple straightforward matter. It is important to recognize that the difficult portion of the problem has been solved for us by modern x-ray instruments. At the same time we should view the remaining task, namely the orientation of the cell, in its proper perspective, and realize that a unique setting is not as significant as it was in the past but is a

matter that should be decided largely by the needs of the problem in hand.

It is evident then that the selection of the conventional unit cell is the most significant point in choosing the setting. Only in unusual circumstances (as in the plagioclases) is it advisable to depart from this convention. The orientation of this cell should be strongly influenced by the special cases of pseudosymmetry, structural analogy, etc. if noteworthy. It is the representation and discussion of these points that enriches mineralogical literature.[1] In the event that no special features are to be emphasized, the setting should aim at being useful to those who study crystals on optical and x-ray goniometers. To the majority of crystallographers this will continue to mean the selection of some direction in the crystal as the "main zone" and its designation as the c axis. The well established conventions α and β obtuse, and $a < b$ should be observed. Even in special cases it is usually advisable to retain at least the custom α and β obtuse if possible. These commonly used conventions are suggested in order to introduce as much uniformity as possible.[2] If no special direction can be singled out, or if a geometrical scheme is to be followed, the choice of c less than a and b is probably the best because it is in accord with the commonest setting.

Appendix

The interpretation of reciprocal lattice projections as plotted from Weissenberg layer photographs is complicated when one of the interaxial angles, either reciprocal or direct, is 90°, or when the negative end of the crystal has been plotted. This is particularly true when morphological information is poorly defined or incomplete. In such cases it may be difficult to determine by inspection, the relative values of the angles with respect to 90° and to locate the positive ends of the axes. It is essential that these circumstances be known before calculation of the direct cell elements can be undertaken. Vandenbrandeite is a special case in that the angle γ^* was measured as 90°0′. As a matter of interest we explored the possible combinations of angles for conventional triclinic cells in which the angles α and β are never acute. This information may be of value to others and therefore is concisely presented here with the aid of a few sketches (Figs. 3–13). In the reciprocal lattice sketches the centre of the projection is shown as a cross. Direct axes are designated a, b and c, while reciprocal axes are shown as H, K and L.

[1] Geometrical rules which do not permit perfect freedom of orientation obviously cannot give adequate expression to these important details.

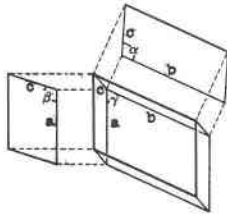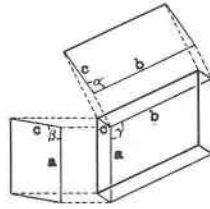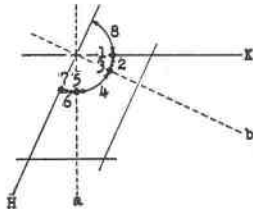[2] Donnay's cyclic permutations are unfortunate because they permit α and β acute, and $b < a$ for the mere sake of having a system.
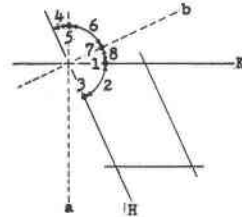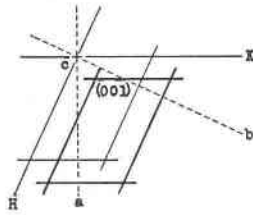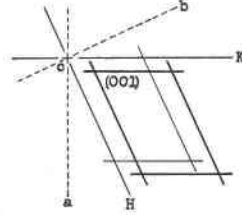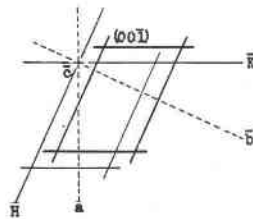
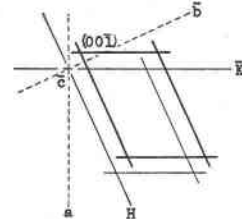FIG. 3

FIG. 4

FIG. 5

FIG. 6

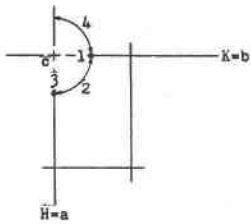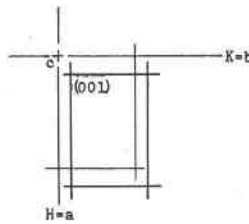FIG. 7

FIG. 8

FIG. 9
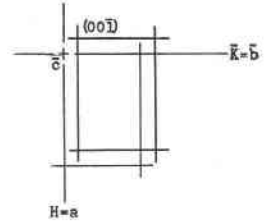
FIG. 10

FIG. 11

FIG. 12

FIG. 13

Figs. 3 and 4 show the two types of oblique triclinic cells. In each case the orientation is chosen so that α and β are obtuse, but in Fig. 3 γ is acute while in Fig. 4 it is obtuse.

In Fig. 5 is represented the $hk0$ layer of the reciprocal lattice for the case in which γ is acute. The numbers 1 to 7 indicate the various positions in which the projection of (001) may fall; for example the reciprocal lattice projection for position 4 is shown in Fig. 7. In position 8 we are dealing with the projection of (00$\bar{1}$), so that c, K and b are negative and γ is obtuse. This is illustrated in Figure 9. The other possible positions of (001) or (00$\bar{1}$) are equivalent to these already indicated and may be brought into coincidence with them by a rotation of 180°. The values of both the reciprocal angles and the direct angles with respect to 90° for each of the 8 positions of (001) of (00$\bar{1}$) are given below.

Position:	1	2	3	4	5	6	7	8
α^*	A[1]	A	A	A	90°	O	O	A
β^*	O	O	90°	A	A	A	A	A
γ^*	O	O	O	O	O	O	O	A
α	O	O	O	O	O	O	90°	O
β	90°	O	O	O	O	O	O	O
γ	A	A	A	A	A	A	A	O

[1] A indicates acute, O obtuse angle.

In Fig. 6 is shown the corresponding diagram for the case in which γ is obtuse. Positions 1, 2 and 3 represent the possible locations of (001), while positions 4 to 8 inclusive represent the positions of (00$\bar{1}$). In the latter locations c, b and K are negative and γ is acute. Figs 8 and 10 illustrate further the angular relations resulting from positions 2 and 6. The relationships of reciprocal angles and direct angles for each of these 8 positions of (001) or (00$\bar{1}$) are given below.

Position:	1	2	3	4	5	6	7	8
α^*	A	A	A	O	90°	A	A	A
β^*	A	A	A	A	A	A	90°	O
γ^*	A	A	A	O	O	O	O	O
α	O	O	90°	O	O	O	O	O
β	90°	O	O	O	O	O	O	O
γ	O	O	O	A	A	A	A	A

Finally in Fig. 11, the case of $\gamma^* = 90°$ has been considered. If the projection of (001) falls in position 1 or 3, there are two right angles in the

unit cell and it is geometrically monoclinic. In position 2 (Fig. 12) the direct cell has 3 oblique angles and in position 4 (Fig. 13) the same applies except that here we are looking at the negative end of the crystal. The angular relations are as follows:

Position 2		Position 4	
α^*—acute	α—obtuse	α^*—acute	α—obtuse
β^*—acute	β—obtuse	β^*—acute	β—obtuse
γ^*—90°	γ—acute	γ^*—90°	γ—acute

ACKNOWLEDGMENTS

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