HEXAGONAL ZONE SYMBOLS AND TRANSFORMATION FORMULAE

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ABSTRACT

Zone symbols in the hexagonal system may be obtained in the usual cross-multiplication manner for three-index symbols by reducing the four-index symbols to three. This is done by adding enough to h, k, and i to reduce one of them to 0. This must be done for both four-index symbols, making the same index 0 in both cases. By dropping this index in both symbols and cross-multiplying, a three-index zone symbol is obtained. This may be changed to a four-index symbol by remembering that h, k, or i is the sum of the other two, multiplied by minus one. The symbol obtained obeys the Weiss zone rule and is the same, regardless of which index was dropped in obtaining the symbol.

Transformation formulae in the hexagonal system are best written as: 1000/0100/0010 /000n, where the only change is in the length of the c axis; or as: 1100/0110/1010/000n, where the first and second order prisms are interchanged, and the length of the c axis may or may not be changed.

Mutual orientation of two crystals of different minerals is best described by noting the parallel crystal planes and the parallel crystal edges of the two species. It is a simple matter to determine these in all but the hexagonal system. The determination of zone symbols in the hexagonal system has not been adequately treated in English or French, and the German writings (Niggli, 1926; Weber, 1922)† seem overcomplicated. Hey (1930) has discussed the problem, but because of a faulty premise in his graphic solution his work is somewhat unsatisfactory. The present paper is an attempt to make available in English a simple procedure for obtaining zone symbols in the hexagonal system.

As is well known, the indices of a line, or edge, or zone are really the coordinates of a point translated certain fractions or multiples of unit distances along two or more coordinates from an origin. In all the crystal systems, save the hexagonal, three coordinates are used to indicate the position of any such point and, thus, the position of the line connecting that point with the origin. This designation may refer to a definite direction and a definite position in space or to only a definite direction. Zone symbols are of the latter type.

In the triaxial crystal systems only one symbol is correct for any given zone. In the hexagonal system, however, which is tetra-axial, there is no unique four-index symbol for designating a particular direction of

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† This paper was written before the German works were discovered, and since the approach and methods were different, it seemed desirable to proceed with publication.

zone. Instead, there are an indefinite number from which, as a matter of convention, one should be chosen.

The heart of the problem lies in an understanding of the relation between symbols based on two and on three horizontal axes. In Fig. 1 it may be seen that the indices which might be ascribed to the point Z are limitless. This is further indicated in Table 1. From these it may be seen that any symbol may be changed without altering its essential correctness by simply adding the same number to h, k, and i of the $hkil$ symbol. Obviously, there is no limit to the numbers which can be added or subtracted.

TABLE 1. VARIOUS POSSIBLE INDICES OF THE POINT Z, FIGS. 1 and 2

$a_1a_2a_3c$	$a_1a_2a_3c$	$a_1a_2a_3c$	$a_1a_2a_3c$
$[\bar{1}\,0\,\bar{3}\,\bar{1}]$	$[0\,1\,\bar{2}\,\bar{1}]$	$[1\,2\,\bar{1}\,\bar{1}]$	$[2\,3\,0\,\bar{1}]$
$+1\,1\,1$	$1\,1\,1$	$1\,1\,1$	$1\,1\,1$
$[0\,1\,\bar{2}\,\bar{1}]$	$[1\,2\,\bar{1}\,\bar{1}]$	$[2\,3\,0\,\bar{1}]$	$[3\,4\,1\,\bar{1}]$
$+1\,1\,1$	$1\,1\,1$	$1\,1\,1$	$1\,1\,1$
$[1\,2\,\bar{1}\,\bar{1}]$	$[2\,3\,0\,\bar{1}]$	$[3\,4\,1\,\bar{1}]$	$[4\,5\,2\,\bar{1}]$
$+1\,1\,1$	$1\,1\,1$	$1\,1\,1$	$1\,1\,1$
$[2\,3\,0\,\bar{1}]$	$[3\,4\,1\,\bar{1}]$	$[4\,5\,2\,\bar{1}]$	$[5\,6\,3\,\bar{1}]$

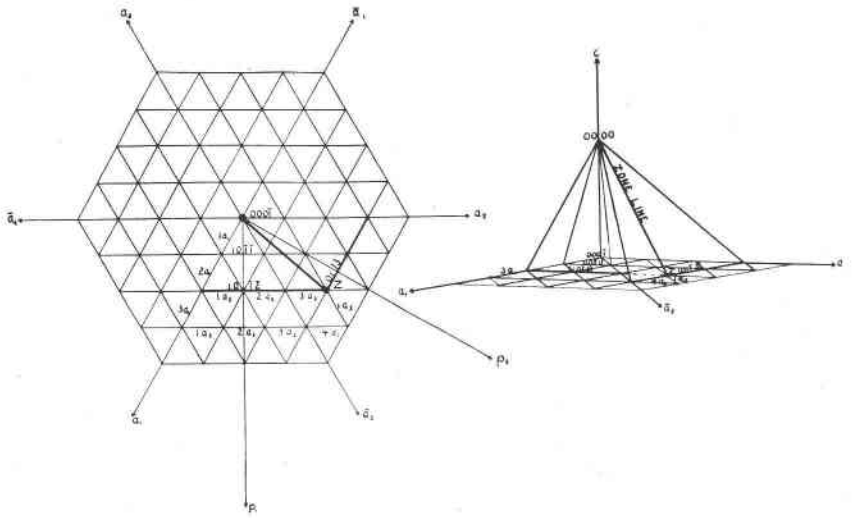

FIG. 1. Hexagonal direct lattice on the plane $c=\bar{1}$, showing the intersection (Z) coordinates of the planes $(10\bar{1}2)$ and $(01\bar{1}3)$.

FIG. 2. Graphic determination of the indices of the edge between $(10\bar{1}2)$ and $(01\bar{1}3)$. For clarification on the plane $c=\bar{1}$, see Fig. 1 and Table 1.

To reduce the *hkil* symbol to a three-index symbol, it is necessary, however, to make h, k, or i equal to zero, not by simply dropping one of them from the four-index symbol, but by adding a number to each that will result in one of these three indices being zero. This means that there are three unique three-index symbols for every point, depending on which combination of the a axes is used. The first step in the determination of a zone symbol is the reduction of the four-index symbol to a three-index symbol as outlined above. Once this has been accomplished the usual cross-multiplication method of obtaining zone symbols is employed. The three-index zone symbol thus obtained is converted to a four-index symbol by the use of the following rule: for the h, k, and i indices, any one of them is the sum of the other two times minus one. The following example will serve to illustrate the procedure.

(1) Determine the three unique three-index symbols for each face (we shall use $(10\bar{1}2)$ and $(01\bar{1}3)$) by adding whatever number is necessary to h, k, and i to reduce each in turn to zero.

	a	b	c	a'	b'	c'
	$10\bar{1}2$	$10\bar{1}2$	$10\bar{1}2$	$01\bar{1}3$	$01\bar{1}3$	$01\bar{1}3$
	$+111$	000	$\bar{1}\bar{1}\bar{1}$	111	$\bar{1}\bar{1}\bar{1}$	000
	2102	$10\bar{1}2$	$0\bar{1}\bar{2}2$	1203	$\bar{1}0\bar{2}3$	$01\bar{1}3$
or	$21/2$	$1/\bar{1}2$	$/\bar{1}\bar{2}2$	$12/3$	$\bar{1}/\bar{2}3$	$/1\bar{1}3$
	$i=0$	$k=0$	$h=0$	$i=0$	$k=0$	$h=0$

(2) Cross multiply three-index symbols for which equivalent indices have been dropped.

	$i=0$			$k=0$			$h=0$		
a	2	1 2 2 1	2	b 1	$\bar{1}$ 2 1 $\bar{1}$	2	c $\bar{1}$	$\bar{2}$ 2 $\bar{1}$ $\bar{2}$	2
a'	1	2 3 1 2	3	b' $\bar{1}$	$\bar{2}$ 3 $\bar{1}$ $\bar{2}$	3	c' 1	$\bar{1}$ 3 1 $\bar{1}$	3
		$\bar{1}$ $\bar{4}$ 3			1 $\bar{5}$ $\bar{3}$			$\bar{4}$ 5 3	
(3) or		$[\bar{1}$ $\bar{4}$ 5 3]			[1 4 $\bar{5}$ $\bar{3}$]			[$\bar{1}$ $\bar{4}$ 5 3]	

The last step is shown just above. It is the conversion of the three-index symbol to a four-index one by making the dropped index equal to the sum of the first two of the three-index symbol times minus one.

Figure 2 demonstrates the correctness of the zone symbol $[14\bar{5}3]$ as determined above. It may be seen that the coordinates of the point Z, which defines the zone symbol, may be $a_1=\frac{1}{3}$, $a_2=4/3$, $a_3=\bar{5}/3$. This figure should be correlated with Fig. 1 to bring out the relations on the plane where $c=\bar{1}$.

Hey (1930) stated that the four-index zone symbol does not obey the Weiss zone symbol rule.* It will be seen that all of the zone symbols

* Namely that with a face $(pqrs)$ in a zone $[hkil]$, the sum of the products $ph+qk+ri+sl=0$.

listed in Table 1 plus the one determined above do obey the rule. Taking two of them at random plus the one above we have:

$(0\ 1\ \bar{1}\ 3)$	$(1\ 0\ \bar{1}\ 2)$	$(1\ 0\ \bar{1}\ 2)$
$\times$	$\times$	$\times$
$[3\ 4\ 1\ \bar{1}]$	$[1\ 2\ \bar{1}\ \bar{1}]$	$[1\ 4\ \bar{5}\ \bar{3}]$
$0+4+\bar{1}+\bar{3}=0$	$1+0+1+\bar{2}=0$	$1+0+5+\bar{6}=0$

Hey's faulty conclusion resulted from an erroneous choice of graphic unit for indexing the intersections on the a_1, a_2, and a_3 axes of the zone line connecting the poles $(10\bar{1}2)$ and $(01\bar{1}3)$. His unit was the distance from the origin to the pole of $(11\bar{2}2)$. The correct graphic unit along the a_1, a_2, and a_3 axes to be used in indexing zone lines is the distance from the center of the projection to the pole of $(11\bar{2}3)$. This is two-thirds of Hey's unit. Figure 3 shows Hey's method of indexing a zone, but the intersection figures given are based on the correct unit. Whereas Hey determined the intersections to be 2, $\frac{1}{2}$ and $\frac{2}{5}$ on a_1, a_2, and a_3 consecutively, the intersections based on the correct unit are 3, $\frac{3}{4}$, and $\bar{3}/5$. Inverting these and making the c intersection equal to $\bar{1}$ we obtain the zone symbol $[14\bar{5}\bar{3}]$ instead of $[14\bar{5}\bar{2}]$ as deduced by Hey.

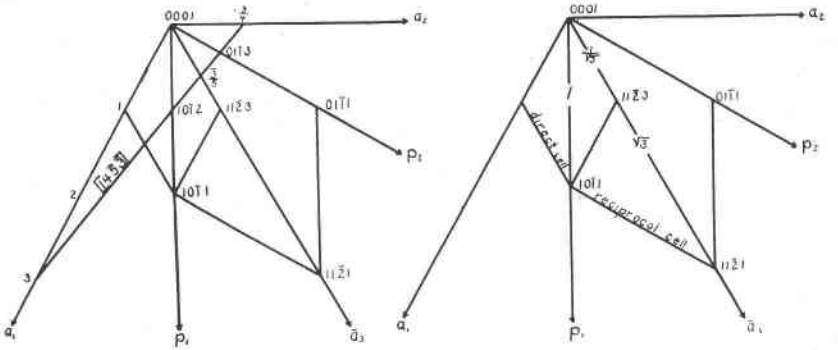

FIG. 3. Gnomonic intercepts on the a axes of the zone line connecting the poles of $(10\bar{1}2)$ and $(01\bar{1}3)$ with unit distance equal to the polar distance of $(11\bar{2}3)$.

FIG. 4. Derivation of the unit length on the a axes for indexing gnomonic zone lines in the hexagonal system.

The choice of $(11\bar{2}3)$ as the unit distance is required by the relation between the reciprocal lattice and the direct lattice in the hexagonal system. Figure 4 shows the reciprocal lattice cell with the face poles which fix it.

If we let the length of the figure's edges be 1, the long diagonal is

equal to $\sqrt{3}$. The reciprocal of 1 is 1, and the reciprocal of $\sqrt{3}$ is $1/\sqrt{3}$, which is one third of $\sqrt{3}$. Thus the correct direct lattice unit along the a axes is one third the length to $(11\bar{2}1)$ or two thirds that to $(11\bar{2}2)$. This is equivalent to the distance from the projection center to the pole of $(11\bar{2}3)$.

Thus, we see that by calculating according to the above method, or by a graphic determination, the same result is obtained. The h/k value of this symbol indicates correctly the phi angle of the zone. This symbol, then, of all the possible symbols, is unique and should be used in the designation of zone symbols in the hexagonal system.

Transformation Formulae

Transformations from the elements of one writer to those of another are usually expressed by means of formulae, the linear type of Barker being commonly used today. In my paper, "Crystallographic Procedures" (1941), I stated in brief the methods for obtaining these formulae but neglected to discuss the special case of the hexagonal system. Two possible choices of axes exist here. The first and second order prisms may be interchanged, and a different unit length for c may be used. To obtain a transformation formula in this system, denote the second order prism faces by the symbols (1000), (0100) and (0010), instead of $(2\bar{1}\bar{1}0)$, $(11\bar{2}0)$ and $(\bar{1}2\bar{1}0)$ by a parallel shift to pass through the origin. Next obtain the equivalence of these in the new orientation.

	(2)	(3)
1000 must equal	$10\bar{1}0$	or $10\bar{1}0$
0100 must equal	0100	or $\bar{1}100$
0010 must equal	0010	or $0\bar{1}10$
0001 must equal	000n	or 000n

Taking the second and third columns and reading the figures vertically we have the two possible transformation formulae in the hexagonal system:

$$1000/0100/0010/000n$$
or
$$1\bar{1}00/01\bar{1}0/\bar{1}010/000n$$

The second formula indicates an interchange of the first and second order prism positions. These formulae, like those in the triaxial systems, permit the ready determination of face indices in the new position and of the new axial lengths. The same procedure as discussed for the triaxial systems applies here.

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