On face- and zone-symbols referred to hexagonal axes.

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THE axial system of Bravais, with three co-planar axes at 120° to one another and a fourth at right angles to them is almost universally adopted for the description of crystals based on the hexagonal prism as unit cell. But it does not seem to have been generally recognized that the use of these axes entails some complications in respect of face- and zone-symbols. These it is the purpose of the present note to consider.

If we take any pair of faces, say $(10\bar{1}2)$ and $(01\bar{1}3)$ and cross-multiply in the usual way, dropping the third index, we obtain a three-index symbol for the zone, $[23\dagger\bar{1}]$. We cannot write in the third index equal to *minus* the sum of the first two, for if we do, the Weiss zone law is only obeyed provided we drop this third index again, a clearly incorrect result. Thus, taking the face $(10\bar{1}2)$, we have: $[23\bar{5}\bar{1}] \times (10\bar{1}2) = 2+0-2 = 0$, but $2+5-2 \neq 0$, and $0+5-2 \neq 0$, and $2+0+5-2 \neq 0$. In fact, the symbol $[23\dagger\bar{1}]$ is complete in itself, and does not include a third index. For convenience, a dagger mark † is used throughout this note to indicate which index is 'absent' in this way; while an asterisk * is used to indicate the position of an index which has been merely 'dropped' for cross-multiplication, &c.

Moreover, if instead of the third we drop the second index and cross-multiply, the zone-symbol becomes $[1\dagger31]$; and if we drop the first index, it becomes $[\dagger1\bar{2}\bar{1}]$.

$$\begin{array}{c|c|c} 1 & 0{*}210 & 2 \\ 0 & 1{*}301 & 3 \\ \hline \multicolumn{3}{c}{[23\dagger\bar{1}]} \end{array} \qquad \begin{array}{c|c|c} 1 & {*}\bar{1}21\bar{1} & 2 \\ 0 & {*}\bar{1}30\bar{1} & 3 \\ \hline \multicolumn{3}{c}{[1\dagger31]} \end{array} \qquad \begin{array}{c|c|c} {*}0 & \bar{1}20\bar{1} & 2 \\ {*}1 & \bar{1}31\bar{1} & 3 \\ \hline \multicolumn{3}{c}{[\dagger1\bar{2}\bar{1}]} \end{array}$$

Finally, we may deduce the zone-symbol from the gnomonic projection by noting the points at which the zone-line cuts the crystallographic axes; or from the linear projection by noting the points at which the normals from the zone-point on to the axes cut the latter. On the gnomonic projection, these points are 2, $\frac{1}{2}$, and $-2/5$ (fig. 1); taking their reciprocals and adding -1 as the unique index, we get [$\frac{1}{2}$, 2, $-5/2$, -1], and clearing the fractions [$14\bar{5}\bar{2}$]. On the linear projection, the points $\frac{1}{2}$, 2, $-2\frac{1}{2}$ give with -1 as fourth index, after clearing of fractions, [$14\bar{5}\bar{2}$]. This time we have obtained a four-index symbol for the zone, and, moreover, one which obeys the rule that each of the first three indices is equal to *minus* the sum of the other two.

Even now the complexities are not exhausted. We rejected the four-index symbol [$23\bar{5}\bar{1}$] derived from [$23\dagger\bar{1}$] by writing in the third index $i = -(h+k)$ because it did not obey the Weiss zone-law. Equally we are compelled to reject the symbols [$1\bar{4}31$] and [$11\bar{2}\bar{1}$] derived similarly from [$1\dagger31$] and [$\dagger1\bar{2}\bar{1}$]. Now the three three-index symbols do obey the Weiss zone-law; but the four-index symbol [$14\bar{5}\bar{2}$], derived from the gnomonic or the linear projection, does not, whether we use all four indices or drop the first, second, or third. It does, however, obey a modified law. The Weiss zone-law is suitable for a three-axis system such as is used in the other crystallographic systems, or obtained by dropping one of the three co-planar axes of the hexagonal system in the above three-index symbols. To make it applicable where there are three co-planar axes we must apply a factor of 3/2 to the unique index, and the zone-symbol [$14\bar{5}\bar{2}$] then obeys this modified law; e. g. taking the face ($10\bar{1}2$), $1+0+5-4\times3/2 = 0$.

The four-index symbol has a simple relation to the three three-index symbols for the zone. If we write the three-index symbols so that they all have the same last index, and then sum them, index for index, taking, however, only 2/3 of the sum for the last index, we have the four-index symbol: $[2-1,\ 3+1,\ -3\ -2,\ 2/3\times(-1)] =$ [$14\bar{5}\bar{2}$].

It is also possible to deduce the three-index symbols from the gnomonic or the linear projection. OA_1, OA_2, and OA_3 are the three co-planar axes (fig. 1); if OA_3 is to be dropped, giving a symbol of the form [$UV\dagger W$], let $O\alpha_1$, $O\alpha_2$ bisect the angles A_1OA_3, A_2OA_3 and take the points where the gnomonic zone-line cuts these special axes, $\frac{1}{2}$, 1/3; take reciprocals, add -1 as third index, and clear of fractions; we then get [$23\dagger\bar{1}$]. Or take the points where the normals from the linear zone-point on these axes cut them, 2, 3; adding -1 as third index, we have [$23\dagger\bar{1}$].

We may now proceed to generalize these relations. Consider two faces $(h, k, \bar{h}+\bar{k}, l)$ and $(p, q, \bar{p}+\bar{q}, s)$; cross-multiplying, we have the three-index symbols $[ql-ks,\ hs-pl,\ \dagger,\ pk-hq]$, $[pl+ql-hs-ks,\ \dagger,\ pl-hs,\ pk-hq]$, and $[\dagger,\ hs+ks-pl-ql,\ ks-ql,\ pk-hq]$. By summation in the above manner we have a four-index symbol $[2ql+pl-2ks-hs, 2hs+ks-2pl-ql, pl-ql-hs+ks, 2pk-2hq]$. The

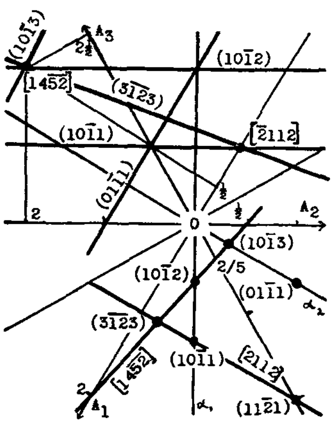

FIG. 1.

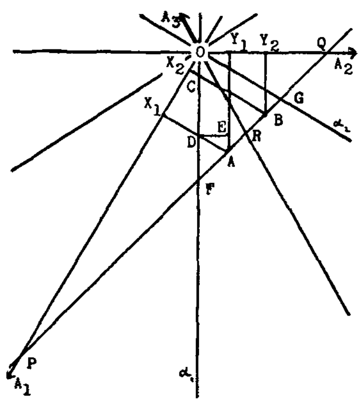

FIG. 2.

FIG. 1. Gnomonic (below) and linear (above) projections showing the derivation of the zone-symbol $[14\bar{5}\bar{2}]$ and the face-symbol $(3\bar{1}\bar{2}3)$. On a radius of projection of 1·25 cm. For [2112] read $[\bar{2}112]$; for $(10\bar{1}3)$ read $(01\bar{1}3)$.

FIG. 2. Gnomonic projection showing the derivation of the four-index symbol for the general zone $[hkil:pqrs] = [A:B]$.

The orientation adopted in these projections is that used by Dana, Groth, Tutton, Lewis, and Miers. A clockwise arrangement of the axes was used by A. Bravais (1851, 1866). V. Goldschmidt has two orientations. For the relation between the hexagonal and rhombohedral axes at least three different methods have unfortunately been in common use.

three three-index symbols obey the ordinary Weiss zone-law; the four-index symbol obeys the modified law given above. For example, taking the face $(h, k, \bar{h}+\bar{k}, l)$:

(i) $hlq+hks-hks-klp+klp-hlq = 0.$

(ii) $hlp+hlq-h^2s-hks-hlp+h^2s-klp+hks+klp-hlq = 0.$

(iii) $hks+k^2s-klp-klq-hks+hlq-k^2s+klq+klp-hlq = 0.$

(iv) $2hlq+hlp-2hks-h^2s+2hks+k^2s-2klp-klq-hlp+hlq$
$+h^2s-hks-klp+klq+hks-k^2s+3/2(2klp-2hlq) = 0.$

We must now ascertain whether the same symbols are derivable from the gnomonic or the linear projection. Let A, B (fig. 2) be any two faces $(h, k, \bar{h}+\bar{k}, l)$ and $(p, q, \bar{p}+\bar{q}, s)$, in gnomonic projection. It is required to find the symbol of the zone-line AB. Let this cut the axes of A_1, A_2, and A_3 at P, Q, and R respectively, then $[1/OP, 1/OQ, -1/OR, -1]$ is the required symbol. Let AX_1, AY_1, AZ_1 be normals from A on the three axes, and BX_2, BY_2, BZ_2 normals from B. Then $OX_1 = h/l$, $OY_1 = k/l$, $OX_2 = p/s$, &c. Now by similar triangles $\dfrac{OP-h/l}{OP-p/s} = \dfrac{PX_1}{PX_2} = \dfrac{AX_1}{BX_2}$. Let OD be a line parallel to AY_1, cutting AX_1 in D, and DE a line parallel to OY_1, cutting AY_1 in E. Then

$$AX_1 = DX_1 + AD = h/l.\tan 30^\circ + DE.\sec 30^\circ = 1/\sqrt{3}.h/l + 2\sqrt{3}.k/l,$$

since DOY_1 is a right angle and angle $A_1OA_2 = 120^\circ$.

Similarly, $BX_2 = 1/\sqrt{3}.1/s.(p+2q)$.

Hence, $$\frac{OP-h/l}{OP-p/s} = \frac{1/\sqrt{3}.1/l.(h+2k)}{1/\sqrt{3}.1/s.(p+2q)},$$
$$(OP-h/l)(lp+2lq) = (OP-p/s)(hs+2ks),$$
$$(lp+2lq-hs-2ks)OP = hp+2hq-hp-2qp,$$
$$\frac{1}{OP} = \frac{2lq+lp-2ks-hs}{2hq-2kp}.$$

Similarly, $$\frac{1}{OQ} = \frac{2hs+ks-2lp-lq}{2hq-2kp}.$$

And since PQR is a straight line and the angles POR, QOR are 60°, OR is a harmonic mean between OP and OQ, that is, $1/OR = 1/OP + 1/OQ$.

Thus the symbol is $[2ql+pl-2ks-hs,\ 2hs+ks-2pl-ql,\ pl-ql-hs+ks,\ 2pk-2hq]$, identical with the above. That the same symbol is also derived from the linear projection is equally readily shown.

The three-index symbols may also be derived from the gnomonic or the linear projection, as outlined above. Taking the general case of fig. 2 again, let QRP cut Oa_1 in F and Oa_2 in G, and let BX_2 cut Oa_1 in C (AX_1 cuts it in D). The required symbol is $[1/OF, 1/OG, \dagger, \bar{1}]$.

By similar triangles, $$\frac{OF-OC}{OF-OD} = \frac{BC}{AD}.$$

We know

$$OC = p/s.\sec 30^\circ,\ OD = h/l\sec 30^\circ,\ BC = q/s.\sec 30^\circ,\ AD = k/l.\sec 30^\circ.$$

Thence, $$\frac{OF-p/s.\sec 30^\circ}{OF-h/l.\sec 30^\circ} = \frac{q/s.\sec 30^\circ}{k/l.\sec 30^\circ},$$

$$OF(k/l - q/s) = kp/sl.\sec 30^\circ - hq/sl.\sec 30^\circ,$$

$$\frac{1}{OF} = \frac{(ks - ql).\sec 30^\circ}{kp - hq}$$

But the unit along Oa_1 is the distance O to $(10\bar{1}1)$ and is $\sec 30^\circ$ times the unit along OA_1, which is O to $(2\bar{1}\bar{1}2)$, so that in terms of the latter unit, $\dfrac{1}{OF} = \dfrac{ks - ql}{kp - hq}$, and $\dfrac{1}{OG} = \dfrac{lp - hs}{kp - hq}$. This gives a symbol $[lq - ks,\ hs - lp,\ \dagger,\ hq - kp]$, identical with the above; and the other three-index symbols are derived similarly.

Between the four symbols of any zone, simple transformation relations may easily be discovered. If the three-index symbol obtained by cross-multiplication in the usual way, omitting the third index, be $[UV\dagger W]$, the other three-index symbols are $[U - V,\ \dagger,\ -V,\ W]$, and $[\dagger,\ V - U,\ -U,\ W]$, and the four-index symbol is $[2U - V,\ 2V - U,\ -U - V,\ 2W]$. Or, if the four-index symbol be $[u,\ v,\ \bar{u} + \bar{v},\ w]$, the three-index symbols are

$$\left[\frac{2u+v}{3},\ \frac{2v+u}{3},\ \dagger,\ \frac{w}{2}\right],\quad \left[\frac{u-v}{3},\ \dagger,\ -\frac{2v+u}{3},\ \frac{w}{2}\right],$$

$$\text{and}\quad \left[\dagger,\ \frac{v-u}{3},\ -\frac{2u+v}{3},\ \frac{w}{2}\right].$$

Consider now the above zone $[14\bar{5}\bar{2}]$ and the zone $[\bar{2}112]$, which may also be written $[10\dagger\bar{1}]$, $[1\dagger0\bar{1}]$, or $[\dagger111]$. By cross-multiplication of their three-index symbols, in the proper pairs, we have the same four-index symbol for the face in each case:

$$\begin{array}{c|c|c} 1 & 0\dagger\bar{1}10 & \bar{1} \\ 2 & 3\dagger\bar{1}23 & \bar{1} \\ \hline \multicolumn{3}{c}{3\bar{1}*3} \\ \multicolumn{3}{c}{(3\bar{1}\bar{2}3)} \end{array} \qquad \begin{array}{c|c|c} 1 & \dagger0\bar{1}10 & \bar{1} \\ 1 & \dagger3113 & 1 \\ \hline \multicolumn{3}{c}{3*\bar{2}3} \\ \multicolumn{3}{c}{(3\bar{1}\bar{2}3)} \end{array} \qquad \begin{array}{c|c|c} \dagger1 & 1111 & 1 \\ \dagger1 & \bar{2}11\bar{2} & \bar{1} \\ \hline \multicolumn{3}{c}{*\bar{1}23} \\ \multicolumn{3}{c}{(3\bar{1}\bar{2}3)} \end{array}$$

But if we cross-multiply the four-index zone-symbols, we obtain a set of three three-index face-symbols, bearing precisely the same relation to one another and to the four-index face-symbol as the three-index zone-symbols do to the four-index zone-symbol.

$$\begin{array}{c|c|c} 1 & 4*\bar{2}14 & \bar{2} \\ \bar{2} & 1*2\bar{2}1 & 2 \\ \hline \multicolumn{3}{c}{(10,\ 2,\ \dagger,\ 9)} \end{array} \qquad \begin{array}{c|c|c} 1* & \bar{5}\bar{2}1\bar{5} & \bar{2} \\ \bar{2}* & 12\bar{2}1 & 2 \\ \hline \multicolumn{3}{c}{(8\dagger\bar{2}9)} \end{array} \qquad \begin{array}{c|c|c} *4 & \bar{5}\bar{2}4\bar{5} & \bar{2} \\ *1 & 1211 & 2 \\ \hline \multicolumn{3}{c}{(\dagger,\ 8,\ 10,\ \bar{9})} \end{array}$$

Then $(10+8,\ 2-8,\ -2-10,\ 9\times 2) = (18,\ \bar{6},\ \overline{12},\ 18) = (3\bar{1}\bar{2}3)$; further $(10,\ 2,\ \dagger,\ 9) = (10-2,\ \dagger,\ -2,\ 9) = (8\dagger\bar{2}9)$, and again $(10,\ 2,\ \dagger,\ 9) = (\dagger,\ 2-10,\ -10,\ 9) = (\dagger,\ 8,\ 10,\ \bar{9})$.

The proof of the generalization of these relations and also of others parallel to those given above for the zone-symbols, to apply to the face-symbols, follows precisely the same lines as for the zone-symbol relations.

It is well known that if $(hkil)$ and $(pqrs)$ are any two faces, then $(mh+np,\ mk+nq,\ mi+nr,\ ml+ns)$ is a third face in the same zone, m and n being any rational numbers. The reciprocal relation of faces and zones in so many respects suggests that it should also hold for the four-index zone-symbols, and it is readily proved that this is the case. For let $[uvtw]$, $[pqrs]$ be two zones. Cross-multiplying, $(qw-vs,\ us-wp,\ \dagger,\ vp-uq)$ is the face common to the two zones. Then if $[mp+nu,\ mq+nv,\ mr+nt,\ ms+nw]$ is a zone passing through this same face, we should have

$$mpqw - mpsv + nquw - nsuv + mqsu - mpqw + nsuv - npvw + mpsv - mqsu + npvw - nquw = 0.$$

As this is true, the relation is proved. A similar relation is easily shown between the three-index symbols of any three co-zonal faces or any three zones having a face in common.

Finally, as we have found the Weiss zone-law to govern the combination of a three-index zone-symbol with a four-index face-symbol or a three-index face-symbol with a four-index zone-symbol, and a simple modification to govern the combination of four-index face- and zone-symbols, we may inquire whether we can find a corresponding relation for the combination of three-index face- and zone-symbols. Such a relation can indeed be found, but it is not so simple as either of the other laws. Consider the pair of faces $(hkil)$ and $(pqrs)$; by cross-multiplication we find that the zone defined by the two faces is $[ks-ql,\ lp-hs,\ \dagger,\ hq-kp]$. And the three-index symbol (with A_3 missing) of $(hkil)$ is

$$\left(\frac{2h+k}{3},\ \frac{2k+h}{3},\ \dagger,\ \frac{l}{2}\right).$$

Combining the two in the ordinary way we have

$$\begin{aligned}
&1/3.(2h+k)(ks-ql) + 1/3.(2k+h)(lp-hs) + \tfrac{1}{2}.l.(hq-kp)\\
&= 2/3.hks + 1/3.k^2s - 2/3.hlq - 1/3.klq + 2/3.klp + 1/3.hlp - 2/3.hks\\
&\qquad\qquad - 1/3.h^2s + \tfrac{1}{2}.hlq - \tfrac{1}{2}.klp\\
&= 1/3.k^2s - 1/3.h^2s - 1/6.hlq + 1/6.klp - 1/3.klq + 1/3.hlp
\end{aligned}$$

$$= 1/3.k(ks-ql) + 1/3.h(lp-hs) + 1/6.klp - 1/6.hlq$$
$$= (ks-ql)(k/3+h/6) - khs/6 + (lp-hs)(h/3+k/6) + khs/6$$
$$= \tfrac{1}{2}\left\{(ks-ql)\left(\frac{2k+h}{3}\right) + (lp-hs)\left(\frac{2h+k}{3}\right)\right\}.$$

That is, after combining the two three-index symbols in the ordinary way, we have an excess equal to half the sum of the products of the first index of each by the second index of the other. In other words, if $(HK\dagger L)$ is a face in the zone $[UV\dagger W]$, then the law corresponding to the Weiss zone-law is $HU+KV+LW-\frac{1}{2}(HV+KU)=0$.

These generalizations, which do not appear to have been previously noticed, show a symmetrical equality of the three co-planar axes, and exhibit the reciprocal relation of zones and faces in a marked degree. And they clear up the apparent contradiction between the zone-symbol as deduced by cross-multiplication, dropping different indices, and as deduced from the gnomonic projection, which has been a source of considerable perplexity to the author from time to time.

The relations may be summed up as follows:

To every face or zone of a crystal referred to the Bravais hexagonal four-axis system there belong four different face or zone-symbols.

Each face-symbol as usually deduced from the gnomonic or the linear projection is the four-index face-symbol in common use.

A four-index zone-symbol may be deduced from the gnomonic or the linear projection, and is not the zone-symbol in common use.

The four-index symbols, both of zones and faces, obey the relation that the sum of the first three indices is zero.

Cross-multiplication of a pair of four-index face- or zone-symbols gives three different zone- or face-symbols according to which pair of indices is dropped before cross-multiplication.

The three-index zone-symbol with third index absent is the zone-symbol in common use, but a system of three-index face-symbols is of no practical use.

These three-index symbols are complete in themselves, and a fourth index cannot be introduced by the rule $i = -(h+k)$.

Cross-multiplication of a corresponding pair of three-index face- or zone-symbols gives, after introduction of the proper index by the rule that the sum of the first three indices is zero, a four-index zone- or face-symbol.

The three-index face- and zone-symbols can also be deduced from the gnomonic projection; if it is proposed to derive the symbol with third index absent, the face-poles and zone-lines are referred to a pair of axes bisecting the angles between $-A_3$, A_1 and $-A_3$, A_2. The linear projection can be similarly treated.

The three-index symbols of any face $(pqrs)$ or zone $[pqrs]$ are

$$\left[\left(\frac{2p+q}{3}, \frac{2q+p}{3}, \dagger, \frac{s}{2}\right)\right], \left[\left(\frac{p-q}{3}, \dagger, -\frac{2q+p}{3}, \frac{s}{2}\right)\right]$$

and

$$\left[\left(\dagger, \frac{q-p}{3}, -\frac{2p+q}{3}, \frac{s}{2}\right)\right].$$

The sign $[(\ )]$ indicating zone or face.

The four-index symbol of any face $(PQ\dagger S)$ or zone $[PQ\dagger S]$ is $[(2P-Q,\ 2Q-P,\ -P-Q,\ 2S)]$, and the remaining two three-index symbols are $[(P-Q,\ \dagger,\ -Q,\ S)]$ and $[(\dagger,\ Q-P,\ -P,\ S)]$.

If the three-index symbols of any face or zone are first written so as to have the same last index, and then summed, index for index, but taking only 2/3 the sum for the last index, the result is the four-index symbol of the face or zone.

If the three-index symbol of a zone or face is combined with the four-index symbol of a face or zone, dropping the appropriate index of the latter, the ordinary Weiss zone-law : $hu+kv+lw = 0$ is satisfied when the face belongs to the zone.

If the four-index symbol of a face $(hkil)$ is combined with the four-index symbol of a zone $[uvtw]$, without dropping any index, a small modification of the Weiss zone-law is necessary, namely $hu+kv+it+\frac{3}{2}\cdot lw = 0$. The factor 3/2 is related to the presence of three co-planar axes.

The law corresponding to the Weiss zone-law governing the combination of a three-index face-symbol (e. g. $(HK\dagger L)$) with a corresponding three-index zone-symbol (e. g. $[UV\dagger W]$) is more complex, namely $HU+KV+LW-\frac{1}{2}(KU+HV) = 0$.

If $(hkil)$ and $(pqrs)$ are any two faces, it is well known that $(mh+np,\ mk+nq,\ mi+nr,\ ml+ns)$ is a co-zonal face, m and n being any rational numbers. A precisely parallel relation holds between the four-index symbols of any three zones having a face in common.

A precisely similar relation also holds between the three-index symbols of any three co-zonal faces or any three zones having a face in common.