A note on crystallographic calculations.

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IN the course of work on the Barker index of determinative crystallo-
graphy, a number of interesting problems have arisen owing to the
selection by a few workers of unusual sets of fundamental angles for
their computations. Most of these problems have been of no general
application, but one appears to have a wider interest and may prove of
practical value in dealing with crystals having curved or striated faces
that only admit of accurate measurements along one zone.

This problem was to compute the angles and elements of a mono-
clinic crystal, using as fundamentals the angles from b (010) to any
three faces e, f, g (of known indices) not in the zone [010], and no pair
of which are co-zonal with b (fig. 1). These fundamentals do not
allow of a solution by spherical triangles, nor by use of the relation[1]
sin cr. tan am.tan bq/sin $ra = 1$ with $ad\ hoc$ axes, as is often possible.

The first step in the solution is to locate by the aid of a sketch gno-
monogram (fig. 2) a zone through any one of the faces (e) which cuts
the zones through b and the other two faces, [bf] and [bg], in faces f', g'
such that the gnomonic intercepts $ef', f'g'$ are equal, a step which is
always possible, and to calculate the angles bf', bg' by the multiple
tangent relation; let this zone, $ef'g'$, cut the zone [010] in a face D (fig. 1),
and let the zones [be], [$bf'f$], [$bg'g$] cut [010] in E, F, and G. Then, since
$EG = DG - DE$,

$$\cos EG = \cos DE . \cos DG + \sin DE . \sin DG$$
$$= (\cot DE . \cot DG + 1) . \sin DE . \sin DG \qquad . \quad \text{(i)};$$

from the triangles Dbe, Dbf', Dbg',

$$\sin D\hat{b}g' = \sin DG = \tan b\hat{D}g' . \cot bg' \qquad . \qquad . \quad \text{(ii)};$$

and $\qquad \cot^2 DG = \operatorname{cosec}^2 DG - 1 = \tan^2 bg' . \cot^2 b\hat{D}g' - 1 \qquad . \quad \text{(iii)}.$

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[1] r (101), m (110), q (011), R (10$\bar{1}$).

Similarly for DE, DF; and as $DEFG$ are a harmonic quartette by construction,

$$2 \cot DF = \cot DE + \cot DG \quad . \quad . \quad . \quad \text{(iv)}.$$

Squaring and rearranging,

$$2 \cot DE \cdot \cot DG = 4 \cot^2 DF - \cot^2 DE - \cot^2 DG$$
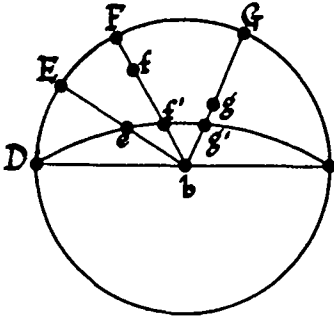$$= (4 \tan^2 bf' - \tan^2 be - \tan^2 bg') \cot^2 b\hat{D}e - 2,$$

FIG. 1.   FIG. 2.
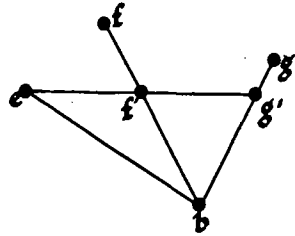
and substituting this in (i) and eliminating sin DE and sin DG by means of (ii), $b\hat{D}e$ cancels out, giving

$$\cos e\hat{b}g = \cos EG = (4 \tan^2 bf' - \tan^2 be - \tan^2 bg')/2 \tan be \cdot \tan bg',$$

which is readily solved. As $e\hat{b}g$ completes a spherical triangle, solution may now proceed on normal lines, but it is usually more convenient[1] to assign temporary indices g' (011), e (110), F (101), D (10$\bar{1}$) and obtain GF, GD' from the relation

$$\cot cr - \cot ca = \cot cR + \cot ca = \tan am \cdot \tan bq \cdot \operatorname{cosec} ca.$$

While the above relation in its most general form only holds for a set of three polar angles measured from a face-pole which is also a zone-axis (as b (010) of a monoclinic crystal), a restricted form is more generally available. For if four poles $Defg$ (fig. 3) form a harmonic quartette and O is the pole of any other zone through D, the above equations hold and connect $e\hat{O}g$ with the angles eO, fO, gO. But as O will not in general be the pole of a face, the relations cannot be extended to any three faces; they must form a co-zonal harmonic quartette with a face (D) in the zone of which O is the pole.

[1] It may perhaps be noted here that if be, bg', eg' (fig. 2) are given as fundamentals, the most direct solution is given by the relation
$$\cot De + \cot eg' = \cos bg'/\cos be \cdot \sin eg'.$$

This extension clearly covers the ρ-angles of three faces (on a crystal measured in zone-adjustment) which form a harmonic quartette with a face in the zone of reference, enabling the ϕ-angles of the three faces to be calculated, and is equally applicable in the anorthic system.
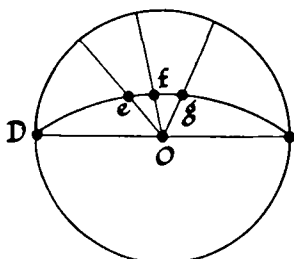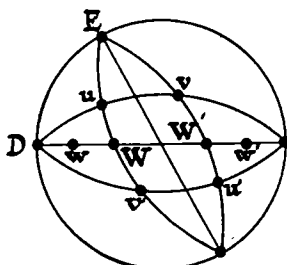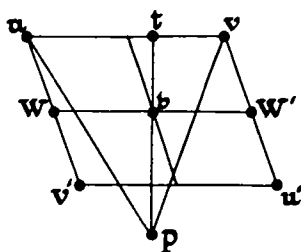
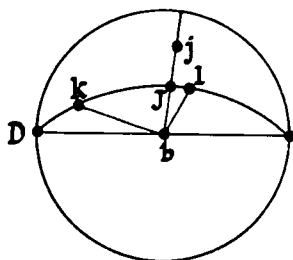

FIG. 3.

FIG. 4.

FIG. 5.

FIG. 6.

Another problem of some interest, though of less general value, is the calculation of the elements of a monoclinic crystal from the angles from a face D in the zone [010] to any two faces, u, v (of known indices) in one zone through D and a third face w in the zone [Db] (fig. 4).[1] Here again it is not possible to solve by spherical triangles in the normal way.[2]

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[1] The measurement of ammonium cobalticyanide by V. von Lang (Sitzungsber. Akad. Wiss. Wien, 1862, vol. 45, Abt. II, p. 107) includes so few angles that the only available fundamentals are of this type. The same selection of fundamentals was made for hydrobromcinchene by W. Muthmann (Zeits. Kryst. Min., 1889, vol. 15, p. 391).

[2] Where the given angles are DW, uW, vW (fig. 4), solution is possible by drawing zone-circles through u and v to cut [DWb] at right angles; the final solution is sec $D\hat{W}u = 2 \cot DW/(\cot uW - \cot vW)$. Unless the angle $D\hat{W}u$ differs considerably from 90°, this selection of fundamentals is very unfavourable, but was used for potassium cobalticyanide by H. Topsøe, Sitzungsber. Akad. Wiss. Wien, 1872, vol. 66, Abt. II, p. 43.

Let the zone $[uv']$ meet $[Dwb]$ in W and the zone $[010]$ in E; the indices of W and the angle DW may readily be calculated. Now let the gnomonic angle point of the zone $[Duv]$ be P and the projection radius of the gnomonic projection (fig. 5) R, and let Pb meet the zone line $[Duv]$ in t. Then $Pt = R.\sec b\hat{D}u = R.\sec b\hat{D}v$, and $P\hat{u}t = Du$, $P\hat{v}t = Dv$. From the plane triangle Put, $ut = Pt.\cot P\hat{u}t = R.\sec b\hat{D}u.\cot Du$, and similarly $vt = R.\sec b\hat{D}u.\cot Dv$. But

$$ut + vt = uv = 2bW = 2R.\cot DW.$$

Hence $\qquad$ $\sec b\hat{D}u = 2\cot DW/(\cot Du + \cot Dv).$

As $b\hat{D}u$ completes a spherical triangle, solution can now proceed on normal lines.

Lastly, one special case in which a simple solution is possible may be mentioned.[1] In a monoclinic crystal, angles from b (010) to any two faces j, k, and the angle kl from one of these faces to a third face not in either of the zones $[bj]$, $[bk]$ are given (fig. 6). If j is not in the zone $[kl]$ let the zones $[bj]$, $[kl]$ cut in J, the indices of which, and the angle bJ, are then calculated; and let the zone $[kl]$ cut $[010]$ in D. Then the anharmonic ratio $\sin Dk.\sin lJ/\sin DJ.\sin lk$ may be calculated; let it be p/q. Now $\cos bk/\cos b\hat{D}k = \sin Dk$, and $\cos bJ/\cos b\hat{D}k = \sin DJ$; substituting in the anharmonic ratio, $\cos bk.\sin lJ/\cos bJ.\sin lk = p/q$, whence lJ may be calculated, and then solution proceeds normally through Dk and the triangle bDk.

[1] Exemplified by 3:3-dimethyl-2-(α-oximinoethyl)-pseudoindol (G. Boeris, cited by P. Groth, Chem. Kryst., 1919, vol. 5, p. 552).