With this formulation none of the minerals contain water molecules as such. The next possible member of the series would have the formula $M_4B_4(SiO_4)(BO_3OH)_3(OH)_4$, and the end-member the formula $M_4B_4(BO_3OH)_4(OH)_4 = MB(BO_3OH)(OH)$.

In herderite, $CaBe(PO_4)(F, OH)$, PO_4 and $BeO_3(F, OH)$ tetrahedra play the same roles as do the SiO_4 and $BO_3(OH)$ tetrahedra in datolite (Pavlov and Belov, 1957).

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SINE TABLE FOR INDEXING POWDER PATTERNS

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The indexing of a line on a powder pattern rests on the comparison of an observed with a calculated quantity, such as the interplanar distance d or some related function.

Tables giving d in Å in terms of θ at every 0.01° (or 2θ at every 0.02°) have been published for the six most commonly used x-ray wave lengths (ref. 1). The calculation of $d(hkl)$, on the other hand, is tedious,[1] even if d is expressed as a function of the reciprocal-cell dimensions a^*, b^*, c^*, α^*, β^*, γ^*.

The easiest function to calculate is

$$Q(hkl) = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2klb^*c^* \cos\alpha^* + 2lhc^*a^* \cos\beta^* + 2hka^*b^* \cos\gamma^* = 1/d^2(hkl),$$

which is the square of the length of the reciprocal-lattice vector. It is probable that, if the powder-data card catalogue could be compiled all

[1] We have in mind the workers who use desk calculators, not the lucky ones who have access to electronic computers.

over again, the Q's rather than the d's would be listed on the cards. At the present time, however, there exists only one table (ref. 2) that gives $Q(2\theta)=\sin^2\theta/(\lambda/2)^2$, *at every 0.01° in* 2θ, but it covers only the range 10° to 70° for copper radiation. This table would have to be extended to higher 2θ values and to all the other useful wave lengths, if Q values were to be listed instead of the customary d's. But until such a decision is reached, and for the more restricted purpose of indexing a pattern, other functions can be used which are independent of wave length and for which tables already exist, for example $(\lambda/2)^2Q(2\theta)=\sin^2\theta$. The reciprocal-cell dimensions must be multiplied by $\lambda/2$ before calculations are performed. Tables of $\sin^2\theta$ are available (ref. 3) for $\theta=0(0.01°)90°$. In precision determinations, 2θ can be read to 0.01°, so that it would be desirable to double the table of $\sin^2\theta$, by taking θ in steps of 0.005°.

Other tables, however, exist which render the extension of the $\sin^2\theta$ table unnecessary, and which require multiplying the reciprocal-lattice lengths by $\lambda/\sqrt{2}$. The function to be used is the versine, for

$$(\lambda^2/2)Q(2\theta) = 1 - \cos 2\theta = \text{vers } 2\theta.$$

The existing tables (ref. 4) of sin x and cos x, for $x=0(0.01°)90°$, can be used simply as follows:

(1) For $2\theta\leq 90°$, let $x=2\theta$, so that vers $2\theta=1-\cos x$; look up cos x and write down its complement to 1.
(2) For $90°<2\theta<180°$, let $x=2\theta-90°$, so that vers $2\theta=1+\sin x$; look up sin x and add it to 1.

Example: if $2\theta=120°$, $x=30°$; you read sin 30°=0.50000 and write 1.50000.

The tables give too many decimal places, but the first five places are separated from the others, so that the tables can easily be used as five-place tables.

It may not be out of order at this point to suggest a mode of presentation for powder data. *All* the lines permitted by the space-group should be calculated from the cell dimensions and should be published. Their purpose is not only to index the lines actually observed on the pattern at hand, but also to help later workers, who, by using longer exposures or other wave lengths, may observe one or more additional lines. Having all *possible* lines on record will make it unnecessary for them to repeat the whole calculation in order to account for the few additional observed lines. In order to cope with the large number of possible lines, it might be advisable, so as to save journal space, to abandon the listing in columns and to print the data as continuous text, with observed values in bold-face type between parentheses after the corresponding calculated values.

Because the quantity that is actually obtained from measurement is

the angle 2θ, we would advocate the recording and comparing of $2\theta_{obs}$ and $2\theta_{calc}$, for the particular wave length used. The $2\theta_{calc}$ values can be read from the sine table once *vers* 2θ has been obtained by calculation. For comparison with the powder-data card catalogue, both d_{obs} (2θ) and d_{calc} (2θ) can then be read from the d-table for the appropriate wave length. Obtaining d_{calc} this way is simpler than deriving it from *vers* 2θ by either formula

$$d = \sqrt{\frac{1}{(2/\lambda^2) \text{ vers } 2\theta}} \quad \text{or} \quad d = \lambda/2 \sin \theta.$$

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