NOTES AND NEWS

GARRELSITE AND THE DATOLITE STRUCTURE GROUP*

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The fact that the *x*-ray powder diffraction patterns of datolite, bakerite, herderite, and homilite are very similar led Frondel (Palache, Berman, and Frondel, 1951) to postulate that a structural resemblance exists among these minerals. He expressed the chemical formulas in the following way:

Datolite	$Ca_4B_4(SiO_4)(SiO_4)_3(OH)_4 = CaB(SiO_4)(OH)$
Bakerite	$Ca_4B_4(BO_4)(SiO_4)_3(OH)_3.H_2O$
Herderite	$Ca_4Be_4(PO_4)(PO_4)_3(F, OH)_4 = CaBe(PO_4)(F, OH)$
Homilite	$(Ca, Fe)_4B_4(SiO_4)(SiO_4)_3(OH)_4 = (Ca, Fe)B(SiO_4)(OH)$ (?)

Recently, Milton, Axelrod, and Grimaldi (1955) described the new mineral garrelsite, $(Ba_{.65}Ca_{.29}Mg_{.06})_4H_6Si_2B_6O_{20}$, and postulated that it also is related to datolite. Following Frondel, these authors write the following chemical formulas:

Datolite	$Ca{\cdot}B_4(SiO_4)_4(OH)_2$
Bakerite	$Ca_4B_4(BO_4)(SiO_4)_3(OH)_3.H_2O$
Garrelsite	$(Ba, Ca, Mg)_4B_4(BO_4)_2(SiO_4)_2(OH)_2.2H_2O$

This way of writing and comparing the formulas implies that the bakerite and garrelsite structures may be derived from the datolite structure by the replacement of one-fourth and one-half, respectively, of the SiO_4 content of datolite, by BO_4, with concomittant decrease in the hydroxyl content in order to maintain the charge balance.

Ito and Mori (1953) have determined the crystal structure of datolite; Pavlov and Belov (1957) have verified their results, and, in addition, have analyzed the crystal structure of herderite. An examination of these crystal structures permits a more detailed assessment to be made of the structural relations existing among all of the minerals listed above. Datolite contains infinite sheets of composition $[BSiO_4(OH)]_n^{-2n}$. In forming a sheet, SiO_4 tetrahedra and $BO_3(OH)$ tetrahedra link at corners so that each SiO_4 shares three corners and has one unshared corner, and each $BO_3(OH)$ shares three corners, with the unshared (OH) at the fourth corner (see Fig. 5 of the paper of Ito and Mori (1953)). Thus, it appears that in deriving bakerite or garrelsite from datolite the SiO_4 should be replaced by $BO_3(OH)$ rather than BO_4. To make this relationship explicit the formulas involved can be written in the following way:

Datolite	$Ca_4[B(OH)SiO_4]_4 = Ca_4B_4(SiO_4)_4(OH)_4$
Bakerite	$Ca_4[B(OH)SiO_4]_3[B(OH)BO_3(OH)] = Ca_4B_4(SiO_4)_3(BO_3OH)(OH)_4$
Garrelsite	$M_4[B(OH)SiO_4]_2[B(OH)BO_3(OH)]_2 = M_4B_4(SiO_4)_2(BO_3OH)_2(OH)_4$ (M = Ba, Ca, Mg)

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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.