

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	$\text{Ca}_4\text{B}_4(\text{SiO}_4)(\text{SiO}_4)_3(\text{OH})_4 = \text{CaB}(\text{SiO}_4)(\text{OH})$
Bakerite	$\text{Ca}_4\text{B}_4(\text{BO}_2)(\text{SiO}_4)_3(\text{OH})_3 \cdot \text{H}_2\text{O}$
Herderite	$\text{Ca}_4\text{Be}_4(\text{PO}_4)(\text{PO}_4)_3(\text{F}, \text{OH})_4 = \text{CaBe}(\text{PO}_4)(\text{F}, \text{OH})$
Homilite	$(\text{Ca}, \text{Fe})_4\text{B}_4(\text{SiO}_4)(\text{SiO}_4)_3(\text{OH})_4 = (\text{Ca}, \text{Fe})\text{B}(\text{SiO}_4)(\text{OH}) (?)$

Recently, Milton, Axelrod, and Grimaldi (1955) described the new mineral garrelsite, $(\text{Ba}_{.65}\text{Ca}_{.29}\text{Mg}_{.06})_4\text{H}_6\text{Si}_2\text{B}_6\text{O}_{20}$, and postulated that it also is related to datolite. Following Frondel, these authors write the following chemical formulas:

Datolite	$\text{Ca}_4\text{B}_4(\text{SiO}_4)_4(\text{OH})_4$
Bakerite	$\text{Ca}_4\text{B}_4(\text{BO}_4)(\text{SiO}_4)_3(\text{OH})_3 \cdot \text{H}_2\text{O}$
Garrelsite	$(\text{Ba}, \text{Ca}, \text{Mg})_4\text{B}_4(\text{BO}_4)_2(\text{SiO}_4)_2(\text{OH})_2 \cdot 2\text{H}_2\text{O}$

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 $[\text{BSiO}_4(\text{OH})]_n^{-2n}$. In forming a sheet, SiO_4 tetrahedra and $\text{BO}_3(\text{OH})$ tetrahedra link at corners so that each SiO_4 shares three corners and has one unshared corner, and each $\text{BO}_3(\text{OH})$ 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 $\text{BO}_3(\text{OH})$ rather than BO_4 . To make this relationship explicit the formulas involved can be written in the following way:

Datolite	$\text{Ca}_4[\text{B}(\text{OH})\text{SiO}_4]_4 = \text{Ca}_4\text{B}_4(\text{SiO}_4)_4(\text{OH})_4$
Bakerite	$\text{Ca}_4[\text{B}(\text{OH})\text{SiO}_4]_3[\text{B}(\text{OH})\text{BO}_3(\text{OH})] = \text{Ca}_4\text{B}_4(\text{SiO}_4)_3(\text{BO}_3\text{OH})(\text{OH})_4$
Garrelsite	$\text{M}_4[\text{B}(\text{OH})\text{SiO}_4]_2[\text{B}(\text{OH})\text{BO}_3(\text{OH})]_2 = \text{M}_4\text{B}_4(\text{SiO}_4)_2(\text{BO}_3\text{OH})_2(\text{OH})_4$ (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).

REFERENCES

- ITO, T., AND MORI, H. (1953), The crystal structure of datolite: *Acta Cryst.*, **6**, 24-32.
 MILTON, CHARLES, AXELROD, J. M., AND GRIMALDI, F. S. (1955), New mineral, garrelsrite, $(Ba_{.65}Ca_{.29}Mg_{.06})_4H_6Si_2B_6O_{20}$, from the Green River formation, Utah: *Geol. Soc. Am. Bull.*, **66**, 1597.
 PALACHE, C., BERMAN, H., AND FRONDEL, C. (1951), *The System of Mineralogy*, 5th Ed., vol. 2, John Wiley and Sons, Inc., N. Y.
 PAVLOV, P. V., AND BELOV, N. V. (1957), Crystal structure of herderite, datolite, and gadolinite: *Doklady Akad. Nauk S.S.S.R.*, **114**, 884-887. [*Chem. Abstr.*, **52**, 176 (1958)].

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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.