# BAVENITE: SYMMETRY, UNIT CELL

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The finding of beryllium in bavenite has led to a new formula.[1] Considerations of symmetry are now clearing up discrepancies in the descriptions of physical properties.

Laue photographs were taken in three rectangular directions. The one with $x$-rays incident along the vertical axis is reproduced in Fig. 1. This, and photographs normal to (100) and (010), showed

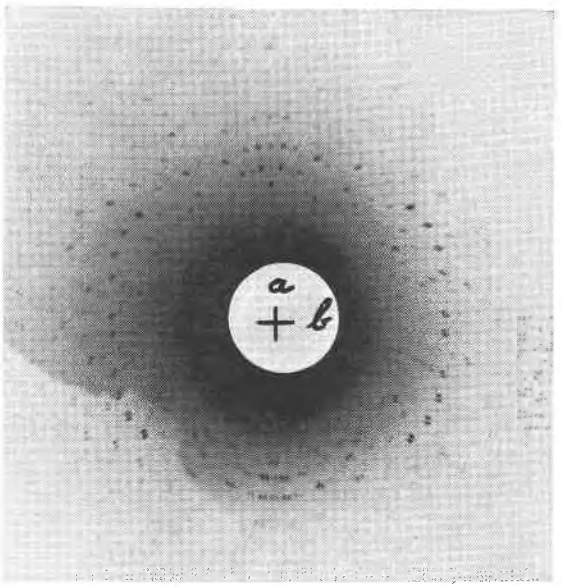


FIG. 1. Laue photograph of bavenite taken with a narrow beam of $x$-rays nearly parallel to the $c$-axis, at a distance of 5 cm. from crystal to plate. Owing to the minute size of the crystal and its composition an extremely long exposure, 58 k.v.–23 m.a., was necessary; a universal type, tungsten anticathode, $x$-ray tube was used.

the two-fold symmetry required of orthorhombic crystals. The obvious doubling of spots accords with goniometric observations kindly made by Dr. George Tunell that vertical striations of the crystal blades are accompanied by slight lack of parallelism of adjoining parts.

[1] W. T. Schaller and J. G. Fairchild, *Am. Mineral.*, **17**, 409, 1932.

Oscillation spectrum photographs were obtained for the same three directions with Cu$-$K$_\alpha$ radiation ($\lambda = 1.538$ Å), from an unstriated crystal about 0.05 mm. thick and 0.3 mm. wide. With the

TABLE 1

FORMS AND ANGLES OF BAVENITE

| New, orthorhombic, orientation | | | | | Old, monoclinic, orientation |
|---|---|---|---|---|---|
| Forms | Calculated | | Observed* | | Forms* |
| | $\phi$ | $\rho$ | $\phi$ | $\rho$ | |
| $a$(100) | 90°00′ | 90°00′ | 90°00′ | 90°00′ | $b$(010) |
| $b$(010) | 0 00 | 90 00 | 2 33 | 90 00 | $a$(100) |
| $m$(110) | 50 0 | 90 00 | 49 29 | 90 00 | $m$(110) |
| $l$(120) | 30 48 | 90 00 | 28 23 | 90 00 | $l$(210) |
| $t$(012) | 0 00 | 12 06 | 0 00 | 11 52 | $c$(001) |
| $u$(032) | 0 00 | 32 46 | 0 00 | 33 57 | $u$(101) |
| $d$(052) | 0 00 | 47 0 | 0 00 | 48 38 | $d$(201) |
| $e$(112) | 50 0 | 18 27 | 52 41 | 19 01 | $e$(012) |

* Adapted from Schaller's table, many of the measurements could be only roughly approximate.

same crystal a rotation photograph and an equator layer-line photograph were taken with a Weissenberg $x$-ray goniometer using Cr$-$K$_\alpha$ radiation ($\lambda = 2.285$ Å), from a metal $x$-ray tube[2] with an interchangeable anticathode. These photographs and accompanying optical and goniometric studies[3] showed no features incompati-

[2] C. J. Ksanda, *Rev. Sci. Instr.*, **3**, 351, 1932.

[3] Slightly inclined and irregular extinctions are seen through cleavage surfaces in the plane of which our measurements show the birefringence of the crystals from Italy to be only 0.0008. Slight strain-birefringence would account for observed irregularities of extinction, especially on different steps of a cleavage face, and the weak birefringence would account for other discrepancies in recorded optical orientation. Narrow whole blades supported edgewise in a liquid of refractive index $\beta$ showed no divisional suture, and only a slight waviness from parallel extinction. (See "Conclusion" for other new measurements.)

A crosswise cleavage on ten blades (Italy) gave a patch of signals about 3° broad normal to the elongation, $c$-axis.

A hypothetical single monoclinic crystal with a beam of $x$-rays incident in any azimuth normal to the $b$-axis would give a Laue pattern of spots symmetrical with respect to the trace of (010), but not with respect to a line parallel to the $b$-axis.

ble with orthorhombic symmetry,[3] therefore calculations for unit cell dimensions, $a_0$, $b_0$, $c_0$, were carried out as shown in Table 2. The corresponding axial ratios are, $a:b:c=0.839:1:0.429$.

TABLE 2

DIMENSIONS OF THE UNIT CELL OF BAVENITE $a_0$, $b_0$, $c_0$, CALCULATED FROM MEASUREMENTS ON FILMS FROM OSCILLATION AND ROTATION PHOTOGRAPHS

| $h, k, l$ | $d/n$ | $a_0$ | $h, k, l$ | $d/n$ | $b_0$ |
|---|---|---|---|---|---|
| (100) | 9.663 | 9.663 | (010) | 11.525 | 11.525 |
| (200) | 4.842 | 9.684 | (030) | 3.846 | 11.538 |
| (300) | 3.219 | 9.657 | (040) | 2.880 | 11.520 |
| (400) | 2.417 | 9.668 | (050) | 2.305 | 11.525 |
| (500) | 1.935 | 9.675 | (060) | 1.922 | 11.532 |
| (600) | 1.612 | 9.672 | (070) | 1.648 | 11.536 |
| (700) | 1.384 | 9.688 | (080) | 1.442 | 11.536 |
| | $a_0=$ | 9.67Å | (090) | 1.283 | 11.547 |
| (001) | 4.949 | $4.95Å=c_0$ | | $b_0=$ | 11.53Å |

By flotation, duplicate measurements of density of four very clear crystals from Italy gave $2.74_5$.

The volume of the unit cell, and the density indicate that one chemical molecule,[1] $9SiO_2 \cdot Al_2O_3 \cdot BeO \cdot 4CaO \cdot H_2O$, is associated with the unit cell of bavenite.[4]

*X*-ray reflections indicate that this unit cell is referable to the simple orthorhombic lattice type $\Gamma_0$, and is isomorphous with one of the space groups $V^1$, $V_h^1$, or $C_{2v}^1$.

A hypothetical pair of monoclinic crystals twinned on (100), the supposed twinning of bavenite (old orientation), would yield a double set of spots having both these elements of symmetry. The zone ellipses through the corresponding spots of the two crystals would be tangent at the center, but because of the inclination of the *a*-axis the two sets would not be spaced properly, except along the *b*-axis, so that it could be interpreted as a set of spots from a single crystal. With rays incident along the *b*-axis the prominent zone ellipses of a hypothetical single monoclinic crystal would have an unsymmetrical distribution of spots, and a twinned pair would yield a general pattern symmetrical with respect to two lines at right angles through the center, but the zone ellipses of one crystal would intersect the corresponding ones of the other. Thus the two sets could not be interpreted as a set from a single crystal.

No analogous double pattern was found on the other types of photographs.

[4] Using mol. wt. = 909.8, and unit mol. wt. $= 1512.1 \times 10^{-24}$ g, the density calculated from *x*-ray data is 2.741.

## Conclusion

Bavenite is here described[5] in a new orthorhombic orientation with $a:b:c=0.839:1:0.429$; unit cell dimensions: $a_0=9.67$ Å, $b_0=11.53$ Å, $c_0=4.95$ Å, with one molecule of $9SiO_2\cdot Al_2O_3\cdot BeO\cdot 4CaO\cdot H_2O$; density $=2.74_5$; habit, blades which are elongated and striated parallel to the $c$-axis and flattened parallel to (010). Several subparallel parts joined edge to edge may have side dome faces in common. Cleavage (100) perfect, (001) fair. Colorless. Optical orientation:[6] $\gamma=a=Bx_a$; $\alpha=c$; $+2V=46°-58°$[5] without notable dispersion; $\beta-\alpha=0.0007$–8, $\gamma-\beta=0.005_0$; $\alpha_D=1.583$–4,[5] $\beta_D=1.585$,[5] $\gamma_D=1.590$.

[5] Original description, E. Artini, *Atti. Acc. Lincei*, **10** (2), 139, 1901. Optical determinations, E. S. Larsen, *Bull. U. S. Geol. Survey*, **679**, 44, 1921. General and detailed descriptions, W. T. Schaller, J. G. Fairchild.[1] The data are from our observations, except $2V=58°$ by Ross[1] on crystals from California. Birefringences were measured directly. Both $\alpha$ and $\beta$ are 0.003 – 0.006, and $\gamma$ is 0.000 – 0.007 higher than previous values.

[6] Dr. Schaller wishes said: "A reexamination of the crystals from Italy shows that the optical orientation as given by me is wrong. The axial plane is parallel to the elongation and to the large face—$a$(100) of the former orientation—essentially as given by Artini."