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# VARIATIONS IN THE UNIT-CELL DIMENSIONS OF TOPAZ AND THEIR SIGNIFICANCE

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## INTRODUCTION

Variations in the optical properties of topaz due to substitution of $OH^-$ for $F^-$ have been known for many years (Penfield and Minor, 1894) and have recently been reviewed by Deer, Howie and Zussman (1962). Although the structure of topaz is well known (Alston and West, 1928; Pauling, 1928) and unit-cell dimensions have been determined for a number of natural samples (Swanson, *et al.*, 1962; Fiedler, 1962), systematic variations in the unit cell dimensions of topaz have not been reported to date. The present investigation concerns variations in the unit-cell dimensions of topaz and their relation to the extent of substitution of $OH^-$ for $F^-$.

## DATA AND THEIR IMPLICATIONS

The unit-cell dimensions and optic axial angles ($2V_\gamma$) of 14 natural samples are given in Table 1.

Unit-cell dimensions were determined from average powder-diffraction data using a Norelco X-ray diffractometer and NaCl as an internal standard. $2\theta$ values for the topaz (320), (031), (211), (220) and (021) X-ray reflections were obtained by averaging four measurements (scan rate $\frac{1}{4}$°/min.) per reflection. $2\theta$ values of the standard reflections

[NaCl (200) and (220)] were determined for CuK$\alpha$($\lambda = 1.5418$ Å) from the unit-cell dimension ($a = 5.6412$ Å at 26°C) given in the International Tables for X-ray Crystallography (1962). Topaz cell dimensions were calculated using a least-squares refinement program at the Computer Center of Washington State University. Significant variations in the unit-cell dimensions of topaz were observed, particularly for *b* (Table 1). Based on two standard deviations ($2\sigma$), the *b* cell dimensions are believed to be known within 0.002 Å for all samples except Nos. 1, 3, 10, ±0.001 Å and No. 11, ±0.003 Å. The precisions of *a* and *c* are equal to or greater than that of *b* for every sample. Unit-cell dimensions of topaz from two localities in Table 1 (Nos. 1 and 2) determined by Swanson *et al.*, (1962) are in close agreement with those obtained in the present study.

TABLE 1. UNIT-CELL DIMENSIONS AND OPTIC AXIAL ANGLES OF NATURAL TOPAZ

| No. | Locality | *a* (Å) | *b* (Å) | *c* (Å) | Volume (Å$^3$) | $2V_\gamma$ |
|---|---|---|---|---|---|---|
| 1. | Durango, Mexico | 8.394 | 8.789 | 4.652 | 343.20 | 68.0° |
| 2. | Topaz Mountain, Thomas Range, Utah | 8.394 | 8.792 | 4.648 | 342.99 | 67.4° |
| 3. | San Luis Potosi, Mexico | 8.396 | 8.794 | 4.651 | 343.40 | 67.0° |
| 4. | Devils Head, Douglas Co., Colorado | 8.394 | 8.801 | 4.655 | 343.89 | 63.6° |
| 5. | Mason County, Texas | 8.394 | 8.803 | 4.652 | 343.75 | 64.0° |
| 6. | Pikes Peak Peg., Lone Lode Claim, Park Co., Colorado | 8.397 | 8.806 | 4.650 | 343.84 | 62.5° |
| 7. | Schneckenstein, Saxony, Germany | 8.393 | 8.807 | 4.652 | 343.86 | 62.5° |
| 8. | China Wall Cupola, Lake George Area, Park Co., Colorado | 8.395 | 8.808 | 4.648 | 343.69 | 63.3° |
| 9. | Brown Derby Mine, Gunnison Co., Colorado | 8.392 | 8.810 | 4.655 | 344.16 | 61.2° |
| 10. | Belowda Beacon, Roche, Cornwall, England | 8.391 | 8.811 | 4.654 | 344.08 | 61.2° |
| 11. | Trumbull, Connecticut | 8.394 | 8.817 | 4.660 | 344.89 | 57.0° |
| 12. | Minas Gerais, Brazil | 8.399 | 8.826 | 4.662 | 345.59 | 53.8° |
| 13. | Ouro Preto, Minas Gerais, Brazil | 8.395 | 8.833 | 4.660 | 345.55 | 51.8° |
| 14. | Brewer Mine, Chesterfield Co., South Carolina | 8.389 | 8.836 | 4.666 | 345.87 | 48.0° |

Optic angle measurements were made in Na-light using procedures described by Emmons (1943). Values given in Table 1 are averages of 15 orthoscopic measurements per sample. Average conosopic measurements for samples 1, 2, and 10 were less than 0.5° greater than those obtained orthoscopically. Optic axial angles (Table 1) are in close agreement with those reported previously for topaz from the same localities (Deer, Howie and Zussman, 1962). The precision of optic angle values is ±1.0° (No. 11, Table 1, ±2.0°) but in view of recent studies by Munro (1963) and others their accuracy is uncertain. Although the optic axial angles determined in this study may not represent absolute values, the relative change in optic angle is believed to be a valid expression of variations in the $OH^-:F^-$ ratio of topaz.

Inspection of Table 1 reveals that the sample (No. 1) with the largest optic angle and, therefore, the smallest $OH^-:F^-$ ratio (Deer, Howie and Zussman, 1962) has the smallest *b* cell dimension. With decreasing optic angle the *b* cell dimension increases progressively for all samples. Since the only major variation in the chemical composition of topaz is in the $OH^-:F^-$ ratio (ibid.), the well-defined inverse relationship between optic angle and *b* (Fig. 1) strongly suggests that *b* is also dependent on this ratio. A similar but weaker correlation exists between small variations in *c* and optic angle (Fig. 2) suggesting that substitution of $OH^-$ for $F^-$ causes a slight increase in *c*; *a* appears to be unaffected by this substitution.

Although chemical analyses were not attempted in the present study, topaz analyses are reported by Deer, Howie and Zussman (1962) for samples from three of the localities in Table 1 (Nos. 2, 10 and 14); optic angle values for these samples are in very close agreement with those obtained in this study. A diagram in which the analytically determined $OH^-/(OH^-+F^-)$ ratios are plotted against *b* is shown in Fig. 3. Additional chemical analyses and unit cell determinations are necessary to establish the relationship between *b* and the $OH^-/(OH^-+F^-)$ ratio with confidence but it is interesting to note than an extrapolation of the curve (Fig. 3) through the three data points to an $OH^-/(OH^-+F^-)$ ratio of zero intersects the *b* axis at 8.789 Å. This value should approximate the *b* cell dimension of fluorotopaz ($Al_2SiO_4F_2$). On the basis of the *b* cell dimension and optic angle topaz from Durango, Mexico (Table 1, No. 1) is believed to lie close to the F-rich end-member.

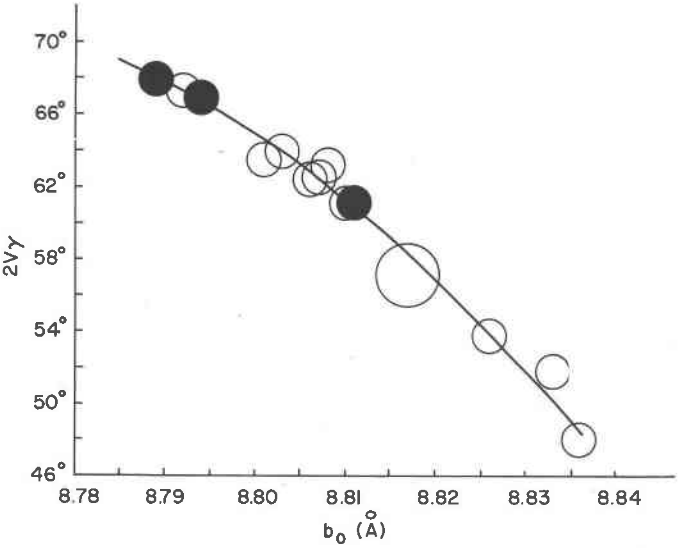

FIG. 1. Variation of *b* cell dimensions with optic axial angles ($2V_\gamma$) of topaz. Diameters of circles approximate or exceed the precision of $2V_\gamma$ and *b*. Filled circles, *b* ±0.001 Å.

## DISCUSSION

Topaz structure is based on a combination of cubic and hexagonal close-packing of oxygen and fluorine atoms which have nearly identical ionic raddi; these anions are arranged in layers parallel to a and c (Alston and West, 1928). The structure is composed of independent silica

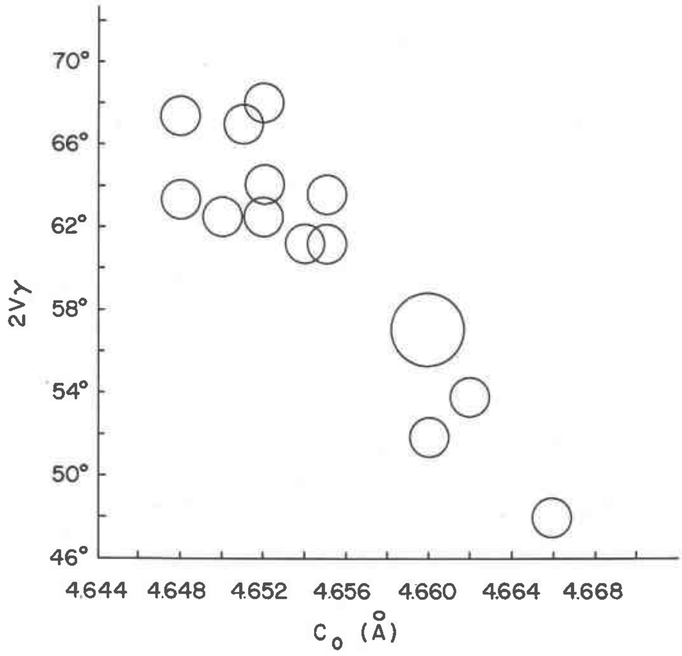

FIG. 2. Variation of *c* cell dimensions with optic axial angles ($2V_\gamma$) of topaz. Diameters of circles approximate or exceed the precision of $2V_\gamma$ and *c*.

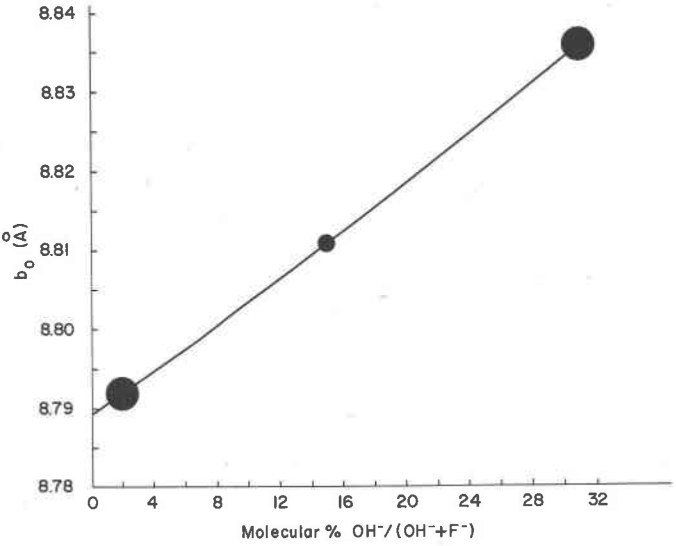

FIG. 3. Variation of *b* cell dimensions (this study) with mole percent $OH^-/(OH^-+F^-)$ of topaz reported by Deer, Howie and Zussman (1962). Diameters of circles approximate the precision of *b*.

tetrahedra and linked octahedral groups around aluminum (Deer, Howie and Zussman, 1962). As a result of the location of fluorine atoms on adjacent rather than opposite corners of the octahedra, alternate layers along the *b*-axis contain; 1) oxygen atoms exclusively, 2) fluorine atoms and oxygen atoms with fluorine predominant.

Substitution of the larger ($\sim$12.5%; Evans, 1964) hydroxyl ion for the fluoride ion should expand the topaz lattice. The presence of alternate oxygen and F-rich layers perpendicular to *b* accounts for the large increase in *b* relative to *a* and *c*. Appreciable expansion of the lattice takes place perpendicular to the anion layers but little or none parallel to these layers. Substitution of $F^-$ for $OH^-$ in phlogopite produces an analogous effect; significant decrease takes place in *c* approximately perpendicular to the mica sheets but little or no change occurs in *a* or *b* which are parallel to the sheets (Yoder and Eugster, 1954).

Since a wide range in $OH^-:F^-$ ratios has been observed, the chemical composition of topaz may be a sensitive indicator of environmental conditions during its formation. It is interesting to note that the three samples (Table 1) with the lowest $OH^-:F^-$ ratios are all from cavities in rhyolites while samples with higher $OH^-:F^-$ ratios are from pegmatites and greisens. When quantitative data are available relating topaz composition to temperature, total pressure and partial pressure of $SiF_4$ (Rosenberg, 1965), the composition of topaz may provide one parameter for delimiting $p$-$T$-$X$ conditions in fluids derived directly from late-stage magmatic environments from which topaz-bearing assemblages are believed to have crystallized.

## CONCLUSIONS

1) The *b* unit-cell dimension of topaz is approximately 8.789 Å for the F-rich end-member and increases progressively with substitution of $OH^-$for $F^-$.

2) Expansion of the topaz structure due to substitution of $OH^-$ for $F^-$ takes place primarily in the *b* unit-cell dimension, perpendicular to the oxygen and F-rich anion layers, which alternate along the *b*-axis.

3) The chemical composition of topaz may be a sensitive indicator of environmental conditions during crystallization of topaz-bearing mineral assemblages.

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# AENIGMATITE FROM THE GROUNDMASS OF A PERALKALINE TRACHYTE

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## INTRODUCTION

Previous chemical analyses of aenigmatite (Fleischer, 1936; Carmichael, 1962; Kelsey and McKie, 1964; Mitrofanov and Afanas'eva, 1966; Zies, 1966) are of phenocrysts from the pantellerites of Pantelleria, the Kola Peninsula, and Greenland, and the alkali syenites of the East Sayan Mts. The aenigmatite reported here is an interstitial mineral in the groundmass of a peralkaline trachyte, and it was analyzed to determine whether there are any significant differences between this type of aenigmatite and that occurring as phenocrysts.

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