

figures. This is certainly better than the accuracy of $\delta(6H)$ since Thibault found no significant difference in δ between different polytypes.

The results are listed in Table 1. The dichroic schemes are typical of only *n*-type (nitrogen-doped) SiC. The colours arise by promotion of free-electrons at the bottom of the conduction band up to higher levels in the conduction bands. (Biedermann, 1965)

The value of δ is insensitive to the concentration of free electrons (typically between 10^{15} – 10^{20} cm^{-3} from Hall effect measurements) and to small additions of boron impurity. Addition of aluminum, however, causes an increase in δ that seems to depend on the number of holes in the valence band if the holes are the dominant free charge carriers.

The value of δ appears, by analogy with ZnS polytypes (Brafman & Steinberger, 1966), to be closely dependent on the proportion, *h*, of hexagonal close-packed planes in the polytype crystal structure (see Fig. 1). There seems to be a tendency for the rhombohedral polytypes to have a slightly lower δ than that of a corresponding hexagonal polytype with the same *h*. The relation suggests that measurement of δ is a valuable preliminary step in determination of an SiC polytype crystal structure.

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REFERENCES

- BIEDERMANN, E. (1965): The optical absorption bands and their anisotropy in the various modifications of SiC. *Solid State Comm.* **3**, 343–346.
- BRAFMAN, O. & STEINBERGER, I. T. (1966): Optical band gap and birefringence of ZnS polytypes. *Phys. Rev.* **143**, 501–504.
- THIBAUT, N. W. (1944): Morphological and structural crystallography and optical properties of silicon carbide. *Am. Mineral.* **52**, 249–278, 327–362.
- VERMA, A. R. & KRISHNA, P. (1966): *Polymorphism and Polytypism in Crystals*, Wiley and Sons, New York.

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FABIANITE AND ITS SYNTHETIC DIMORPH, $\text{CaB}_8\text{O}_5(\text{OH})$: NEW DATA*

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The structure and other crystallographic properties of the synthetic compound $\text{CaB}_8\text{O}_5(\text{OH})$ were reported by Clark *et al.* (1962). At nearly

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the same time, Kühn *et al.* (1962) published a crystallographic description of the new mineral fabianite, also of composition $\text{CaB}_3\text{O}_5(\text{OH})$.

We have determined the space group and unit-cell parameters of fabianite, and have redetermined the optical properties and crystal habits of both dimorphs. The present results are compared with those of the previous investigators in Table 1 and in the text. Indices of refraction of the dimorphs were determined by the immersion method in sodium light using a spindle stage similar to that described by Wilcox (1959). Indices of refraction of the immersion media were determined with an Abbé refractometer using sodium light. Measurements of $2V$ and the relationships between principal optic axes of symmetry and crystallographic axes of reference were obtained using a four-axis universal stage and Waldmann sphere with single crystals oriented by optical goniometry and x -ray precession photography. The specific gravity of fabianite was determined by means of a Berman balance.

In comparing our results with those of Kühn *et al.* (1962), we reoriented their crystal setting by interchanging their a and c axes. Our results are in reasonably good agreement with theirs (Table 1) except that a rotation of 45° in (010) is required to bring the two optical orientations into coincidence.

The optical data given in Table 1 for synthetic $\text{CaB}_3\text{O}_5(\text{OH})$ represent a substantial refinement of those provisionally reported by Clark *et al.* (1962). Similarly, the x -ray powder data presented in Table 2 are more detailed and precise than those given by Kühn *et al.* (1962).

Principal forms of two crystals of synthetic $\text{CaB}_3\text{O}_5(\text{OH})$ determined by optical goniometry are {110}, {120}, {130}, and {010}, and one crystal is terminated by {142} and the other by {552}. Clark *et al.* (1962) reported the terminal form {111}. The $a:b:c$ ratio 0.7960:1:0.6261 determined for fabianite by Kühn *et al.* (1962) is incorrect; the x -ray results of the present study yield the ratio 0.6286:1:0.6069. The difficulty of exact measurement by optical goniometry due to striations and growth irregularities is mentioned by Kühn *et al.* (1962, p. 287).

Tennyson (1963) suggested the possibility that the structure of searlesite, $\text{NaBSi}_2\text{O}_5(\text{OH})_2$, might be related to that of synthetic $\text{CaB}_3\text{O}_5(\text{OH})$. The structure of searlesite has since been solved by Kravchenko (1964), and it is clear from a comparison of the published figures for the two structures (Fig. 1, Clark *et al.* 1962; Fig. 4, Kravchenko 1964) that the two structures are not closely related. Infrared data obtained on fabianite by Kühn & Moenke (1963) indicate that the mineral contains borate tetrahedra and borate triangles.

During editing of the manuscript of this paper the crystal structure of fabianite was determined by Judith A. Konnert and Joan R. Clark,

TABLE 1. X-RAY CRYSTALLOGRAPHIC AND OPTICAL DATA FOR FABIANITE AND $\text{CaB}_3\text{O}_6(\text{OH})$

Symmetry Space Group $a(\text{\AA})$ b c β $V(\text{\AA}^3)$ $d(\text{calc.}) \text{ gm/cm}^{-3}$ Spec. grav. (meas.) Cell contents α β γ Optic sign $2V(\text{obs.})$ Optic orientation ^o	Fabianite		$\text{CaB}_3\text{O}_6(\text{OH})$	
	Present study	Kühn <i>et al.</i> (1962) ^a	Present study	Clark <i>et al.</i> (1962)
	Monoclinic $P2_1/a$	Monoclinic	Orthorhombic	Orthorhombic $Pbmn_2$
	6.593 ± 1^b			6.972^c
	10.488 ± 2			13.47
	6.365 ± 1			4.891
	$113^{\circ}23' \pm 1'$	$113^{\circ}10'$		(90°)
	401.1 ± 1			412.4
	2.788	2.796^d		2.729
	$2.77 \pm 1(25^{\circ}\text{C})$			2.72 ± 1
	$4[\text{CaB}_3\text{O}_6(\text{OH})]$			$4[\text{CaB}_3\text{O}_6(\text{OH})]$
	$1.612 \pm 2(22^{\circ}\text{C})$	$1.608(22^{\circ}\text{C})$	$1.608 \pm 2(25^{\circ}\text{C})$	
	$1.636 \pm 2(22^{\circ}\text{C})$	$1.638(22^{\circ}\text{C})$	$1.616 \pm 2(25^{\circ}\text{C})$	
	$1.653 \pm 3(22^{\circ}\text{C})$	$1.650(22^{\circ}\text{C})$	$1.640 \pm 2(25^{\circ}\text{C})$	
	$(-)$	$(-)$	$(+)$	$(-)$
	$67^{\circ} \pm 2^{\circ}$	64.7°	$55^{\circ} \pm 2^{\circ}$	
	$Y = b$	$Y = b$	$X = c$	$X = b$
	$X \wedge a = +22^{\circ} \pm 2^{\circ}$	$X \wedge a = -23.3^{\circ}$	$Y = a$	$Y = c$
	$Z \wedge c = -45^{\circ} \pm 2^{\circ}$	$Z = c$	$Z = b$	$Z = a$

^aOriginal crystal setting of Kühn *et al.* reoriented to agree with setting of present work.

^bCell constants obtained from least-squares refinement of powder data using the computer program of Evans *et al.* (1963). In all cases the listed error applies to the last digit, *i.e.*, 6.593 ± 1 means 6.593 ± 0.001 .

^cCell constants $\pm 0.3\%$ (Clark *et al.*, 1962).

^dProbably too high because of included anhydrite in sample used.

^eAn extinction angle is given as positive if it is measured to a position in the acute angle between a and c , and negative if it is measured in the obtuse angle.

TABLE 2. X-RAY DIFFRACTION DATA FOR FABIANITES^a

<i>hkl</i>	<i>d</i> (Å)calc.	<i>d</i> (Å)obs.	<i>I</i> / <i>I</i> ₀	<i>hkl</i>	<i>d</i> (Å)calc.	<i>d</i> (Å)obs.	<i>I</i> / <i>I</i> ₀	<i>hkl</i>	<i>d</i> (Å)calc.	<i>d</i> (Å)obs.	<i>I</i> / <i>I</i> ₀
001	5.843	5.86	8	$\bar{2}02$	2.706			$\bar{1}13$	2.073	2.074	54
020	5.244	5.248	33	040	2.622			$\bar{3}12$	2.053	2.052	33
110	5.242			$\bar{2}20$	2.621	2.620	48	203	2.049		
011	5.104	5.118	17	$\bar{2}12$	2.620			241	2.045		
111	4.809			022	2.552			$\bar{3}21$	2.024	2.025	56
120	3.963	3.962	54	131	2.494	2.493	25	142	2.020	2.020	37
021	3.903	3.904	27	140	2.406	2.406	37	$\bar{2}13$	2.011		
121	3.766	3.766	21	$\bar{2}22$	2.404						
111	3.369			041	2.392						
$\bar{2}01$	3.268	3.269	100	$\bar{2}31$	2.388						
211	3.120			141	2.360						
$\bar{1}12$	3.033	3.032	83	$\bar{1}32$	2.348						
130	3.027			201	2.336						
200	3.026			230	2.288						
031	3.000	3.000	23	211	2.280	2.280	10				
121	2.944			112	2.245						
131	2.936			032	2.242	2.242	40				
002	2.922	2.920	87	$\bar{3}11$	2.148	2.148	25				
210	2.908			$\bar{2}32$	2.140						
012	2.814	2.815	27	221	2.134	2.135	19				
$\bar{2}21$	2.774	2.777	8	141	2.111						
122	2.712	2.711	12	122	2.105	2.105	25				

^a Diffractometer chart X-3221; Cu/Ni, CuK α_1 = 1.5405 Å; Si internal standard; scanning speed 1/4° 2 θ /min.; chart scale 1° 2 θ /in.; 1° divergence slit; 1° scatter slit; 0.003 in. receiving slit; *d*(calc.) for *d*_{hkl} ≥ 2.000 based on lattice parameters given in Table 1. The pattern also showed a few lines due to anhydrite impurity; these lines are not included above.}

U.S. Geological Survey (oral communication). Fabianite contains the same $[\text{B}_3\text{O}_5(\text{OH})]_n^{-2n}$ sheets found in the synthetic $\text{CaB}_3\text{O}_5(\text{OH})$, but in fabianite the Ca is eightfold coordinated, in contrast to the sixfold coordination determined in the synthetic dimorph (Clark *et al.*, 1962). The resulting closer packing accounts for fabianite having a smaller cell volume and greater density than the synthetic compound.

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REFERENCES

- CLARK, J. R., CHRIST, C. L., & APPLEMAN, D. E. (1962): Studies of borate minerals (X): The crystal structure of $\text{CaB}_3\text{O}_5(\text{OH})$. *Acta Cryst.* **15**, 207–213.
- EVANS, H. T., JR., APPLEMAN, D. E., & HANDWERKER, D. S. (1963): The least-squares refinement of crystal unit cells with powder diffraction data by an automatic computer indexing method; (abstr.). *Am. Cryst. Assoc., Cambridge, Mass., Ann. Meet. Program*, 42–43.
- KRAVCHENKO, V. B. (1964): The crystal structure of searlesite, $\text{NaBSi}_2\text{O}_5(\text{OH})_2$. *Soviet Physic Cryst.* **9**, 143–148.
- KÜHN, R., ROESE, K. L., & GAERTNER, H. (1962): Fabianit $\text{CaB}_3\text{O}_5(\text{OH})$, ein neues Mineral. *Kali u. Steinsalz* **3**, 285–290.
- KÜHN, R. & MOENKE, H. (1963): Ultrarotspektroskopische Charakterisierung des neuentdeckten Borminerals Fabianit $\text{CaB}_3\text{O}_5(\text{OH})$ und seines Begleiters Howlith. *Kali u. Steinsalz* **3**, 399–400.
- TENNYSON, CH. (1963): Eine Systematik der Borate auf kristallchemischer Grundlage. *Fortschr. Mineral.* **41**, 64–91.
- WILCOX, R. E. (1959): Use of the spindle stage for determination of principal indices of refraction of crystal fragments. *Am. Mineral.* **44**, 1272–1293.

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THE OPTICAL ABSORPTION SPECTRUM OF TETRAHEDRALLY BONDED Fe^{3+} IN ORTHOCLASE

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Recently there has been much interest in the effect of Fe^{2+} and Fe^{3+} on the optical absorption spectra of silicate minerals and on the structural implications of such spectra (*e.g.*, Burns, 1965; White and Keester, 1966;

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