Groups about Be(III), Be(IV), and Be(V) atoms are the final bits of inter-rod 'glue' encountered along ⟨111⟩ directions before diverging rods leave large (5·4 Å diameter) holes centered at sites such as 0, 0, 0 and 1, 1, 1. Some indication of the manner in which these groups interlock with the rod structure may be seen in Fig. 4.

Hole configuration

The large inter-rod holes are relatively isolated from one another. They are surrounded by the square bases of Ca(II)O_6 groups in ⟨100⟩ directions, by the prism sides of Ca(I)O_8 groups in ⟨110⟩ directions, and by triangular faces of Be(IV)O_4 and Be(V)O_3 groups in ⟨111⟩ directions. The shortest path between them is through a Ca(I)O_8 group; a more devious path lies through a Be(V)O_3 group, into a $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$ pocket, and into an adjoining large hole through another Be(V)O_3 group.

Structural obstacles along either path would seem to dictate low interhole diffusion rates for large guest atoms or molecules. This has been tentatively verified by repeated failures in attempts to introduce argon into the holes by treating calcium beryllate in a 2400-lb.in^{-2} argon atmosphere at 500 to 550°C for periods up to 18 hr. Diffusion rates may be higher for small atoms or molecules (He or H_2), and the possible entrapment of guest atoms during formation of calcium beryllate is worth investigation.

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References

Ader, M. & Bingle, J. (1956). Argonne National Laboratory, Chemical Engineering Div. Quart. Progr. Rep. April–Juni, p. 106.

Busing, W. R., Martin, K. O. & Levy, H. A. (1962). *A Fortran Crystallographic Least-Squares Program.* Oak Ridge National Laboratory, Tennessee. ORNL TM-305.

Busing, W. R., Martin, K. O. & Levy, H. A. (1964). *A Fortran Crystallographic Function and Error Program.* Oak Ridge National Laboratory, Tennessee. ORNL TM-306.

Cromer, D. T. & Waber, J. T. (1964). Los Alamos Scientific Laboratory, New Mexico. LA-3056.

Farrell, E. F., Fang, J. H. & Newnham, R. E. (1963). *Amer. Min.* **48**, 804.

Harris, L. A., Potter, R. A. & Yakel, H. L. (1962). *Acta Cryst.* **15**, 615.

Howells, E. R., Phillips, D. C. & Rogers, D. (1949). *Research,* **2**, 338.

Howells, E. R., Phillips, D. C. & Rogers, D. (1950). *Acta Cryst.* **3**, 210.

Hughes, E. W. (1941). *J. Amer. Chem. Soc.* **63**, 1737.

International Tables for X-ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press.

Marezio, M., Plettinger, H. A. & Zachariasen, W. H. (1963). *Acta Cryst.* **16**, 390.

Pauling, L. & Shappell, M. D. (1930). *Z. Kristallogr.* **75**, 128.

Pavlov, P. V. & Belov, N. V. (1960). *Soviet Phys., Crystallography,* **4**, 300.

Potter, R. A. & Harris, L. A. (1962). *J. Amer. Ceram. Soc.* **45**, 615.

Smith, D. K., Newkirk, H. W. & Kahn, J. S. (1964). *J. Electrochem. Soc.* **111**, 78.

Smith, D. K., Cline, C. F. & Austerman, S. B. (1964). U.C.R.L. 7539, Rev. 1.

Warren, B. E. (1930). *Z. Kristallogr.* **74**, 131.

Wilson, A. J. C. (1942). *Nature, Lond.* **150**, 152.

Acta Cryst. (1966). **20**, 301

The Crystal Structure of Bavenite

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Bavenite, a silicate containing aluminum, beryllium, calcium and hydrogen, is orthorhombic, with space group *Cmcm*, $Z=4$, $a=23·19$, $b=5·005$, $c=19·39$ Å. Its crystal structure has been solved from a three-dimensional Patterson synthesis. Final bond lengths and angles were determined from coordinates obtained by the least-squares method applied to three-dimensional data (final over-all R value: 6·6 %). Bavenite displays a framework-like structure in which the dominant motif is a fourfold chain of linked tetrahedra running parallel to **b**. The diadochy between aluminum, tetrahedrally coordinated, and beryllium is discussed. The positions of the hydrogen atoms have been determined and an improved chemical formula has been derived, *i.e.* $Ca_4(BeOH)_{2+x}Al_{2-x}Si_9O_{26-x}$, where $0·10 \leq x \leq 0·84$.

Introduction

Bavenite is a silicate containing aluminum, beryllium and calcium, always found in a tardomagmatic environment. After some discussion it has been recognized as orthorhombic. Its probable space group is reported as *Cmcm* and slightly varying lattice constants have been found by different authors who handled different specimens (Berry, 1963). It often occurs in

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* G.F. carried out the differential thermal analysis of bavenite, contributing to the arrangement of the chemical formula.

plates normal to [100], elongated following [010], very narrow in the [001] direction. The cleavages are {001} very good, {100} good. The chemical analyses were discussed by Berry (1963), who suggested

$$H_xCa_4Be_{2+x}Al_{2-x}Si_9O_{27} \,.\, nH_2O \quad (0{\cdot}10 \le x \le 0{\cdot}84; \quad n=1{\cdot}08)$$

as the correct chemical formula.

Experimental

Chemical formula

One of us (G.F.) carried out a differential thermal analysis of bavenite. This showed that the latter loses water only at 950° with decomposition, and the chemical formula can therefore perhaps better be written

$$H_{2+x}Ca_4Be_{2+x}Al_{2-x}Si_9O_{28} \quad (0{\cdot}10 \le x \le 0{\cdot}84).$$

The reported chemical formula, with this minor variation, was assumed to be correct, without making a new analysis; the results of the crystal structure determination were consistent with all the assumptions made. Our specimens from Baveno had an atomic ratio $Al:Be \simeq 1{\cdot}9:2{\cdot}1$.

Lattice constants

The lattice constants were determined at room temperature by measuring the 2θ-values of appropriate reflexions for each of the constants to be determined, and extrapolating the corresponding interplanar distances, plotted against $\frac{1}{2}\left(\frac{\cos^2\theta}{\sin\theta}+\frac{\cos^2\theta}{\theta}\right)$, to $2\theta=180°$. The measurements were made with a Wooster single-crystal diffractometer. The values so obtained are as follows:

$$a=23{\cdot}19\pm0{\cdot}02\ \text{Å}$$
$$b=5{\cdot}005\pm0{\cdot}009$$
$$c=19{\cdot}39\pm0{\cdot}02$$
$$U=2250{\cdot}5\ \text{Å}^3$$

Space group: *Cmcm*; $Z=4$.

Recording of intensities

An approximate crystal structure was determined from Weissenberg and precession intensities from two crystals not very suitable for refinement work; actually the Patterson and first Fourier maps were accomplished with the use of this first recording. When a better bavenite specimen became available, a new and more accurate recording of intensities was made for refinement purposes. The following discussion is concerned with this latter recording.

The specimen was a narrow plate elongated in the **b** direction. Its dimensions along **a** and **c** were respectively 0·065 mm and 0·049 mm.

The crystal was mounted about the *b* axis, and Weissenberg equi-inclination integrating and non-integrating photographs were obtained for reciprocal lattice levels from $k=0$ to $k=4$, using nickel-filtered copper radiation and the multiple-film technique. The integration range was adjusted to correct for the spot contraction at the higher levels; this correction did not cover a few reflexions elongated rather than contracted on the side of the 'contraction effect' (130, 131, 240, 241, 041).

A total of 1162 independent reflexions out of the 1361 present in the Cu $K\alpha_1$ limiting sphere (85%) was inspected; 66 did not give observable blackening on the films.

Measurement of the intensities

The highest intensities ($I_{obs}>750$, on the absolute scale) were measured on the integrated films with a Nonius microdensitometer and the lowest (one fourth of the whole) were visually estimated by comparison of the non-integrated spots with a calibration strip recorded with a suitable bavenite reflexion. Only an octant of the Cu $K\alpha$ limiting sphere was examined.

Correction and scaling of intensities

The intensities were corrected for Lorentz-polarization and absorption factors, elongation of some spots, and incipient but incomplete $\alpha_1-\alpha_2$ spot doubling. A secondary extinction correction and a correction to all the visual readings were applied at an advanced stage of the refinement (see *Refinement*).

A modification of Albrecht's method (Smith, 1959) was applied for the absorption correction; the linear absorption coefficient of bavenite is $\mu=143$ cm.$^{-1}$ for Cu $K\alpha$ and the transmission factors varied from 0·32 to 0·57. The elongation of some spots, listed above, was corrected approximately by an estimate of the relative areas of the spots. The correction suggested by Sakurai (1962) was applied for the $\alpha_1-\alpha_2$ splitting effect, with the replacement of Υ for θ (Buerger's notation) in the interpolation formula.

The intensities for the different levels were on approximately the same scale owing to the similar exposure times. At first they were separately placed upon an absolute scale by Wilson's method; after each structure-factor calculation, the scale was improved by the criterion $\Sigma F_o=\Sigma F_c$, applied separately to each level.

Structure analysis

Patterson sections were computed at $v=0$, $v=\frac{1}{4}$ and $v=\frac{1}{8}$; only the first is reported here (Fig. 1); it is equivalent to the section at $v=\frac{1}{2}$ with the origin translated by $a/2$ along the u axis.

A model of the arrangement of the cations was constructed on the basis of these considerations:

(1) Owing to the diadochy between Al and Be, it is very probable that the Al atoms resemble the Be and Si atoms in being tetrahedrally coordinated.

(2) The ratio between the numbers of tetrahedrally coordinated atoms (*T* atoms) and the oxygen atoms is 13:28, which strongly suggests a three-dimensional framework for bavenite.

(3) The Patterson section at $v=\frac{1}{2}$ shows a peak at $(u, w)=(\frac{1}{15}, 0)$ corresponding to a distance of 3 Å; this peak, labelled P in Fig. 1 (referred to $v=\frac{1}{2}$), and the translation $b=5{\cdot}005$ Å are consistent with the existence of pyroxene-like chains along [010] with T atoms lying on the plane (001).

(4) The very short b unit translation forbids superimpositions of atoms along [010] in one unit cell, and greatly limits the possibilities of multiple occupation of special positions.

(5) The Patterson section at $v=0$ is a Harker section (Fig. 1); in particular, since the maximum M_1 with coordinates (u_0, w_0) related to those of M_2 $(u_0, 0)$ and M_3 $(0, w_0)$, is very high, it is probably due to Ca–Ca distances, with $u_0=2x_{Ca}$ and $w_0=\frac{1}{2}-2z_{Ca}$.

(6) Many maxima of the above Patterson section can be arranged in pairs pseudo-centrosymmetrically with respect to $(u, w)=(\frac{1}{4}, \frac{1}{4})$. This is consistent, in this space group, with distances between equivalent atoms at $y=\frac{1}{4}$ or $y=\frac{3}{4}$. The maxima labelled M can be correlated in this way with those labelled M'. The y coordinates of the calcium atoms are therefore probably near to $\frac{1}{4}$ and $\frac{3}{4}$.

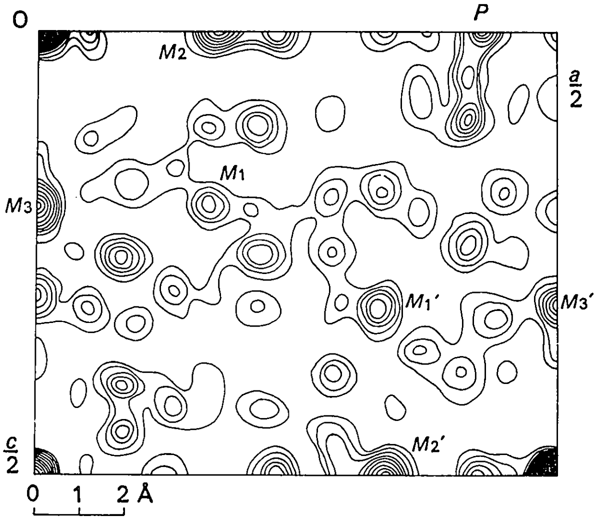

Fig. 1. Patterson section normal to [010]; $v=0$. Contours are drawn at equal but arbitrary levels of density. The Patterson section at $v=\frac{1}{2}$ is obtained by translating the origin by $a/2$ along the u axis. M_1, M_2, M_3: maxima related to the vectors Ca–Ca; M_1', M_2', M_3': maxima related to the preceding ones by a pseudocenter of inversion at $(u, w)=(\frac{1}{4}, \frac{1}{4})$; P: maximum that is related in the section $v=\frac{1}{2}$ to distances between tetrahedrally coordinated cations within chains running parallel to **b**.

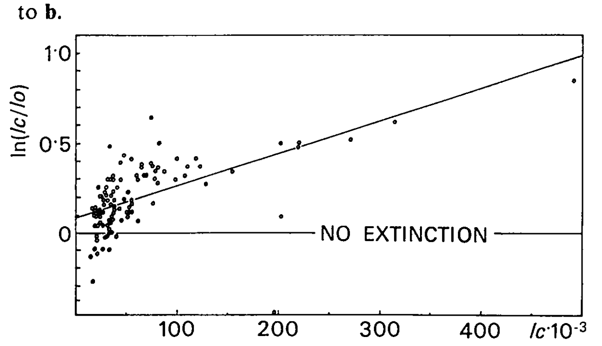

Fig. 2. Plot of ln I_c/I_o against I_c . 10^{-3} for the 102 most intense reflexions, before correction for the secondary extinction effect. The inclined straight line was obtained by the least-squares method applied to the equation $\ln I_c/I_o=\varepsilon I_c+\varepsilon'$. It will be seen that ε' is quite low; the number of reflexions taken into consideration is therefore high enough.

The construction of the model started from the calcium atoms which were arranged in general positions as suggested by (5) and (6), and with four equivalent silicon atoms disposed at (c) (*International Tables* notation), with symmetry *mm*, this last requirement being imposed by the fact that the unit cell contains 36 silicon atoms, while the multiplicities of the general positions are 16 and those of the special positions are 8 and 4. These were labelled $T(1)$. In Fig. 3(f) one sixteenth of the unit cell is roughly schematized to show the only symmetry elements of interest in this discussion. In accordance with (2), $T(2)$ and $T(3)$ were placed on mirror planes at (g) and (f) respectively; testing of the distances Ca–$T(1)$, Ca–$T(3)$ and Ca–$T(2)$ on the Patterson sections was successful for the first two, but negative for Ca–$T(2)$, suggesting therefore that $T(2)=$ Be. Following (4), the positions on the mirror planes were considered to be fully occupied and those on binary axes were first tested seeking for distances between Ca and T atoms on diads; so $T(4)$ and $T(5)$ were found at $y=0$ and $y=\frac{1}{2}$ respectively, or *vice versa*, developing a chain along [010] as stated in (3). Following (4) again, the remaining sixteen T atoms should lie on a general position, $T(6)$, whose coordinates are suggested by Fig. 3(f) in view of completing the connection of the T atoms in a six-membered ring. $T(6)$ is near to the b-glide plane, so developing a new chain along [010] similar to that just described.

The correctness of the model was well verified by an electron density projection along [010] performed with the signs given by the cations only; it gave the approximate x and z oxygen coordinates. The approximate y coordinates of the T atoms were established during the search for the Ca–T vectors on the Patterson sections and by spatial considerations. Those of the oxygen atoms were found paying attention to the tetrahedral coordination of the T atoms and to the connection between these tetrahedra and the calcium coordination polyhedron, which must comply with the third Pauling's rule.

A structure factor calculation with the above coordinates gave an overall R value of 0·30 ($R=\Sigma||F_o|-|F_c||/\Sigma|F_o|$).

Refinement and assessment of accuracy

The method of least squares was applied in order to minimize the unweighted differences F_o-F_c. The calculations were carried out on an Elea 6001 digital computer with a program that takes into account the full matrix; the structure factors were derived starting from the atomic scattering factors obtained from Moore's (1963) constants. At first six cycles were accomplished assuming an isotropic temperature factor for each atom; the progress of the refinement was indicated by a fall in the R value from 0·300 to 0·099.

At this stage the F_o's corresponding to the visual readings were separately compared with the F_c's and an overestimating factor of 1·22 was found; since this value appeared to be independent of the level under consideration, it was explained as a systematic error in the scaling between the integrated and the non-integrated films, and its reciprocal was applied as a correction to all the visual readings.

Moreover a plot of $\ln I_c/I_o$ against I_c for the 102 most intense reflexions pointed out a conspicuous secondary extinction effect (Fig. 2). A search for correl-

Table 1. *Atomic coordinates and their standard deviations*

(fractional standard deviations in parentheses)

Atom	x/a	y/b	z/c	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
Ca	0·0842(1)	0·2425(4)	0·1524(1)	0·0023 Å	0·0020 Å	0·0019 Å
$T(1)$	0·0000	0·7802(5)	0·2500		0·0025	
$T(2)$ = Be	0·1252(4)	0·8218(25)	0·2500	0·0093	0·0125	
$T(3)$	0·0000	0·7227(5)	0·1047(1)		0·0025	0·0019
$T(4)$ = Al	0·0958(1)	0·5000	0·0000	0·0023		
$T(5)$	0·1704(1)	0·0000	0·0000	0·0023		
$T(6)$	0·2141(1)	0·8539(5)	0·1428(1)	0·0023	0·0025	0·0019
O(1)	0·0000	0·5769(11)	0·1830(2)		0·0055	0·0039
O(2)	0·0000	0·0302(10)	0·1139(2)		0·0050	0·0039
O(3)	0·0572(2)	0·5976(14)	0·0718(2)	0·0046	0·0070	0·0039
O(4)	0·1314(2)	0·2298(13)	0·0361(2)	0·0046	0·0065	0·0039
O(5)	0·2081(2)	0·8636(13)	0·0598(2)	0·0046	0·0065	0·0039
O(6)	0·2337(2)	0·5575(12)	0·1646(2)	0·0046	0·0060	0·0039
O(7)	0·1547(2)	0·9245(12)	0·1799(2)	0·0046	0·0060	0·0039
O(8)	0·1211(2)	0·4868(13)	0·2500	0·0046	0·0065	
O(9)	0·0586(2)	0·9504(12)	0·2500	0·0046	0·0060	

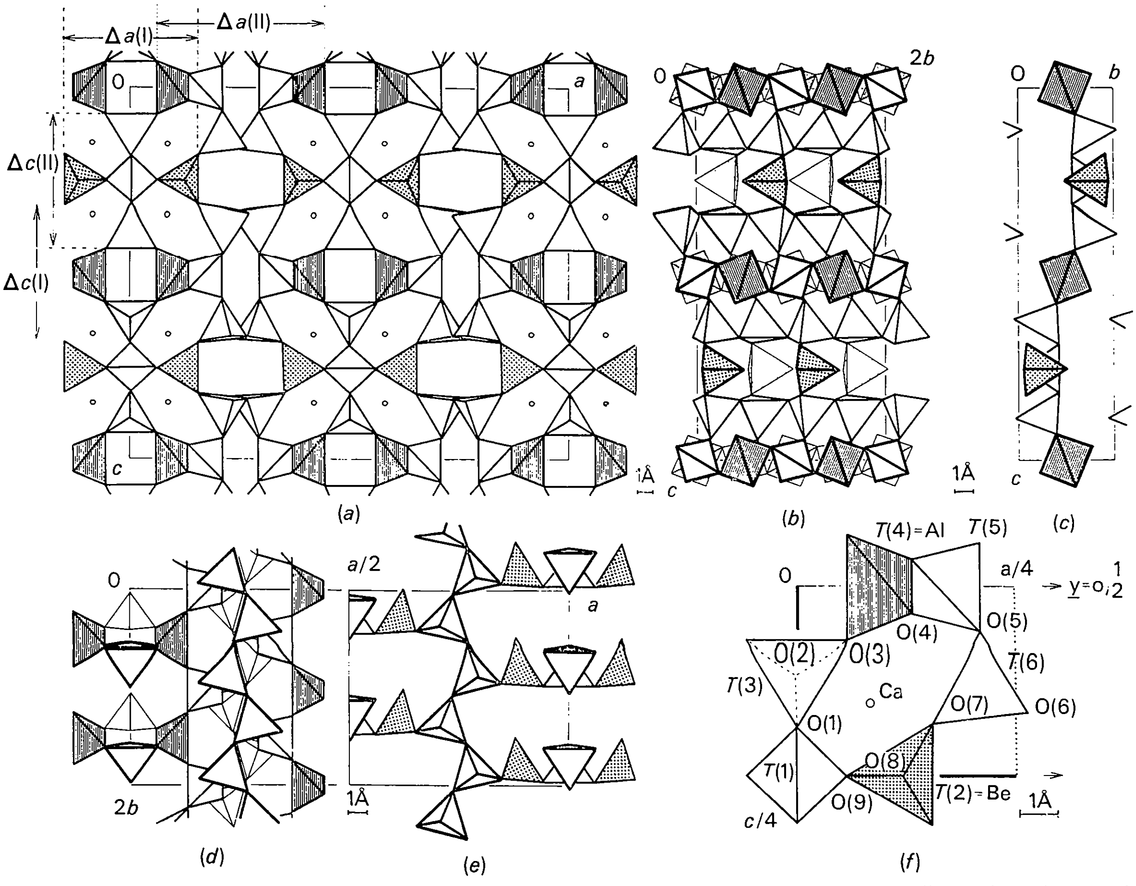

Fig. 3. The crystal structure of bavenite. (*a*) Projection along **b** of the whole unit cell and its surroundings. (*b*) and (*c*) Projections along **a** of cell slabs defined by Δa(II) and Δa(I) respectively; note the lengths of the projection sides. (*d*) and (*e*) Projections along **c** of cell slabs defined by Δc(I) and Δc(II) respectively; note the lengths of the projection sides. (*f*) Projection of one sixteenth of the unit cell and key to the identification of the atoms; the symmetry elements of interest are roughly schematized.

ation between this effect and the θ angle or the crystal shape (Hamilton, 1957) did not give significant results. A linear relation between ln I_c/I_o and I_c was assumed and a least-squares secondary extinction coefficient derived. This was applied as a correction to all the F_o's through the formula $(F_o)_{corr}=(F_o)_{ext}\,.\,\exp\,(\frac{1}{2}\varepsilon I_c)$, where $\varepsilon=2{\cdot}47\,.\,10^{-6}$.

The above corrections lowered the *R* value to 0·074. Two anisotropic least-squares cycles followed. At this point the refinement was considered complete. The final *R* value for 1162 F_{hkl} reflexions, including the unobserved ones, was 0·066.

The atomic parameters and their standard deviations (Cruickshank, 1949) are listed in Table 1. The anisotropic thermal parameters are shown in Table 2. The observed and calculated structure factors are compared in Table 3.

Table 2. *Analysis of anisotropic thermal parameters: root mean square thermal vibrations along the ellipsoid axes* (Å), *magnitudes of the principal axes* (Å^2) *and angles* (°) *between the crystallographic axes and the principal axes of the vibration ellipsoids*

Atom	r.m.s.	B_i	α	β	γ
Ca	0·12	1·08	0	90	90
	0·15	1·70	90	7	83
	0·11	0·89	90	83	173
T(1)	0·10	0·75	90	90	0
	0·12	1·17	90	0	90
	0·07	0·43	0	90	90
T(2) = Be	0·12	1·05	112	22	90
	0·16	2·07	22	68	90
	0·11	0·90	90	90	0
T(3)	0·10	0·86	0	90	90
	0·13	1·36	90	0	90
	0·09	0·60	90	90	0
T(4) = Al	0·10	0·86	0	90	90
	0·13	1·28	90	2	88
	0·10	0·75	90	88	178
T(5)	0·09	0·64	0	90	90
	0·14	1·47	90	3	87
	0·09	0·60	90	87	177
T(6)	0·09	0·64	6	84	90
	0·12	1·10	96	6	90
	0·09	0·60	90	90	0
O(1)	0·10	0·85	90	55	145
	0·13	1·29	0	90	90
	0·08	0·56	90	35	55
O(2)	0·13	1·29	0	90	90
	0·15	1·90	90	0	90
	0·11	1·05	90	90	0
O(3)	0·14	1·56	132	57	121
	0·16	2·04	57	34	80
	0·10	0·82	121	80	33
O(4)	0·12	1·18	137	52	106
	0·15	1·71	58	38	71
	0·11	0·95	65	85	154
O(5)	0·12	1·07	113	70	31
	0·14	1·60	65	27	99
	0·11	0·94	145	73	119
O(6)	0·11	1·04	120	75	146
	0·15	1·68	93	19	71
	0·10	0·80	30	79	118
O(7)	0·12	1·06	41	87	49
	0·13	1·43	110	28	72
	0·11	0·96	56	62	133
O(8)	0·13	1·31	107	17	90
	0·14	1·50	90	90	0
	0·10	0·82	17	73	90
O(9)	0·11	0·94	85	4	90
	0·12	1·20	90	90	0
	0·09	0·64	175	85	90

Discussion

Interatomic distances and angles are presented in Table 4, as well as their standard deviations (Ahmed & Cruickshank, 1953; Darlow, 1960). Reference has to be made to Fig. 3(*f*) in order to identify the labelled atoms.

Identification of the tetrahedral cations

T(1), *T*(3), *T*(5) and *T*(6) were readily identified as silicon atoms, on the basis of their average distances from the surrounding oxygen atoms (1·626, 1·608, 1·613 and 1·614 Å respectively) and of their numbers of electrons, which were estimated to be approximately 12·1, 11·3, 12·2 and 11·8 by integration of the three-dimensional Fourier maxima. *T*(2) has about 1·8 electrons and was therefore identified as beryllium; the average *T*(2)–O distance (1·641 Å) is consistent with this assumption. Finally, the average *T*(4)–O distance (1·729 Å) was decisive for recognizing *T*(4) as aluminum; this atom had 11·2 electrons.

Distances and coordination polyhedra

The Al–O distances are remarkably short; the Al–Be diadochy can account in part for this feature, as the Be:Al ratio slightly exceeds the theoretical ratio of 1:1.

The *T*–O distances of the tetrahedra *T*(2) (= Be) and *T*(3) (= Si) are somewhat irregular; attention has to be paid to the fact that both these tetrahedra correspond to the only interruptions in the three-dimensional framework of tetrahedra, on O(8) and O(2) respectively [Fig. 3(*f*)]. The distance *T*(2)–O(8) is quite long, while the distance *T*(3)–O(2) is shorter than any other *T*–O distance. According to the chemical formula suggested by Berry, one atom of hydrogen accompanies every atom of beryllium, and it is likely to be linked to O(8), since without the hydrogen, this would point towards an empty domain and would have a lower coordination number than the other oxygen atoms of this tetrahedron. It is true that these last features are the same for O(2) relatively to *T*(3); however, one atom of hydrogen linked to O(2) would increase the positive charge around the latter excessively (Table 5), which is not consistent at all with the noticeable shortness of the distances of O(2) from the positive atoms linked to it, *i.e.* *T*(3) and Ca.

Ca–O distances are shown in Table 4 in order of increasing length. The six shortest Ca–O distances vary between 2·34 and 2·51Å; the next longest distance, Ca–O(1), differs from the preceding one by nearly 0·13 Å. There is a weak electrostatic interaction between Ca and O(1) because O(1) is screened by the other oxygen atoms. Therefore the coordination number of calcium can be taken as 6, excluding O(1), or as 6+1. Its coordination polyhedron resembles a trigonal prism with bases O(2)O(3)O(4) and O(7)O(8)O(9), but it is

Table 3. *Structure factors of bavenite*

Reflexions marked with a dot were unobservably weak; in this case F_{obs} derives from 0·5 I_{min}. Some reflexions are not tabulated here; they are 11 reflexions cut off at high θ angles, and 10 reflexions trapped by the direct beam stop. Furthermore the 127 *h5l* and 51 *h6l* reflexions, out of the equiinclination range, are not taken into consideration.

k	l	$10F_o$	$10F_c$
0 k l			
4	1	385	360-
0	2	306	172-
4	2	278	339
2	3	649	564-
4	3	236	216-
0	4	1827	2008-
2	4	2943	2848
4	4	910	880
2	5	284	254-
4	5	376	327
0	6	3424	3422
2	6	367	215
4	6	1111	1073
2	7	137	140-
4	7	80	79-
0	8	1442	1562
2	8	146	136
4	8	1683	1733
2	9	1445	1484
4	9	230	197-
0	10	3124	3350-
2	10	2623	2814
4	10	483	458
2	11	827	787-
4	11	627	670
0	12	3165	3223
2	12	1437	1376
4	12	1200	1204
2	13	915	901-
4	13	460	462
0	14	1000	1065
2	14	110	111
4	14	402	348-
2	15	48·	66-
4	15	205	273-
0	16	629	506
2	16	2540	2659
4	16	437	436-
2	17	784	812
4	17	431	407-
0	18	173	168
2	18	1103	1118
4	18	789	804
2	19	918	897-
4	19	109	102-
0	20	2486	2582
2	20	929	889-
2	21	175	139
0	22	191	175-
2	22	1061	990
2	23	856	852
0	24	438	446-
1 k l			
3	0	588	549-
3	1	2623	1687
3	2	206	185
1	3	302	286-
3	3	590	525
1	4	435	406-
3	4	694	640-
1	5	1932	2078
3	5	1067	1059-
1	6	239	220
3	6	555	557-
1	7	1872	2030-
3	7	2061	2073
1	8	755	756
3	8	300	280-
1	9	1657	1767-
3	9	562	573
1	10	496	521-
3	10	893	887
1	11	507	604
3	11	1555	1617-
1	12	485	528-
3	12	296	317-
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2	0	1521	1700
4	0	756	722-
2	1	294	344
4	1	423	390-
0	2	90	74
2	2	49·	50
4	2	318	291
2	3	296	352-
4	3	166	142-
0	4	451	486
2	4	159	172-
4	4	1166	1073
2	5	527	492-
4	5	378	313
0	6	1286	1341-
2	6	1473	1581
4	6	1072	990-
2	7	51·	24-
4	7	369	338-
0	8	888	886
2	8	51·	56
4	8	501	472
2	9	1046	1050
4	9	361	290-
0	10	1163	1205
2	10	905	967-
4	10	1462	1341
2	11	296	305-
4	11	405	361
0	12	526	504
2	12	742	681
4	12	90	84
2	13	285	287-
0	14	573	539-
2	14	929	845
2	15	389	300
0	16	1629	1617
2	16	456	354-
2	17	141	170
0	18	24·	9
2	18	104	141
19 k l			
1	0	1124	1099
3	0	558	270-
1	1	2296	2303
3	1	552	492-
1	2	736	746-
3	2	99	97-
1	3	1282	1286
3	3	361	321-
1	4	639	645-
3	4	127	149
1	5	858	852-
3	5	606	572
1	6	418	414
3	6	392	388-
1	7	310	312
3	7	130	148
1	8	208	217
3	8	170	175-
1	9	1279	1299
3	9	889	826-
1	10	840	893-
3	10	557	526
1	11	985	987-
3	11	58	49
1	12	39·	49
3	12	144	126
1	13	210	189-
3	13	491	465-
1	14	70	117-
3	14	987	912-
1	15	616	545
3	15	477	450-
1	16	30·	22
1	17	234	196-
1	18	100	103-
20 k l			
0	0	498	453
2	0	296	334
4	0	333	256-
2	1	47·	7-
4	1	102	115
0	2	41·	57
2	2	70	55
4	2	92	98-
2	3	244	260-
4	3	27·	6
0	4	158	91-
2	4	289	308-
4	4	121	126-
2	5	123	135
4	5	371	342-
0	6	1120	1150-
2	6	880	887
4	6	505	427-
2	7	436	401
4	7	57	60-
0	8	410	400-
2	8	475	452-
4	8	491	453
2	9	47·	50
4	9	91	89-
0	10	1119	1097
2	10	517	468-
4	10	424	465
2	11	179	194-
0	12	38·	45
2	12	194	209-
2	13	119	121
0	14	892	867-
2	14	445	367
2	15	119	144-
0	16	1012	905
2	16	293	249-
0	18	426	380
21 k l			
1	0	1590	1692-
3	0	423	409
1	1	128	126-
3	1	204	194-
1	2	859	821-
3	2	667	621-
1	3	254	316-
3	3	415	353-
1	4	40·	28-
3	4	1355	1300-
1	5	665	712
3	5	83	105-
1	6	1476	1469-
3	6	674	577-
1	7	562	555-
3	7	743	698
1	8	450	384-
3	8	31·	51-
1	9	758	713-
3	9	220	266-
1	10	214	200-
3	10	1060	972-
1	11	512	464
3	11	284	257-
1	12	704	680-
3	12	794	748-
1	13	1086	1062
3	13	103	105
1	14	1124	1122-
1	15	752	716-
1	16	427	374-
1	17	301	303-
22 k l			
0	0	1482	1492
2	0	846	893-
4	0	1362	1373
2	1	690	706-
4	1	272	253-
0	2	125	99
2	2	517	508
4	2	273	250
2	3	464	449-
4	3	458	435
0	4	404	370-
2	4	412	413
4	4	419	379-
2	5	311	338
4	5	18·	48
0	6	630	579
2	6	279	270
4	6	295	330
2	7	400	412-
4	7	259	193-
0	8	883	877
2	8	176	187-
2	9	41·	36
0	10	136	104
2	10	794	717
2	11	139	170
0	12	503	489
2	12	94	112-
2	13	52	25
0	14	344	337-
2	14	582	512
2	15	128	187
0	16	706	606-
23 k l			
1	0	868	761
3	0	627	536-
1	1	58	69-
3	1	197	188
1	2	479	444
3	2	515	489
1	3	68	65-
3	3	351	313
1	4	463	336-
3	4	287	295
1	5	451	416
3	5	838	754-
1	6	271	405
3	6	107	96-
1	7	1290	1226-
3	7	912	801
1	8	643	643
3	8	94	120-
1	9	162	162-
3	9	890	790
1	10	414	358-
3	10	1014	1068
1	11	588	526
3	11	206	447-
1	12	28·	82
1	13	24·	18-
1	14	865	818
1	15	585	596-
24 k l			
0	0	2507	2648
2	0	1529	1531-
2	1	375	389
0	2	110	87-
2	2	632	563
2	3	396	327
0	4	932	909-
2	4	1102	978
2	5	40·	12-
0	6	706	665
2	6	373	314-
2	7	37·	82
0	8	1183	1106
2	8	223	189-
2	9	389	354
0	10	1063	995-
2	10	1350	1190
2	11	688	673-
0	12	264	231
2	12	457	405-
0	14	455	419
25 k l			
1	0	37·	56-
3	0	215	220
1	1	444	364-
3	1	154	154
1	2	719	642
3	2	425	417
1	3	284	284-
3	3	137	117-
1	4	215	199
3	4	508	492-
1	5	1211	1088
3	5	987	963-
1	6	31·	20
3	6	511	481
1	7	592	522-
3	7	893	1004
1	8	195	204-
1	9	745	722-
1	10	614	570
1	11	847	781
1	12	19·	42
26 k l			
0	0	408	414-
2	0	704	661-
2	1	611	587-
0	2	1419	1405-
2	2	473	424-
2	3	429	373-
0	4	849	806-
2	4	575	491-
2	5	752	667
0	6	387	379-
2	6	28	5
2	7	60	49
0	8	548	520-
2	8	954	949-
2	9	594	617-
0	10	292	183
0	12	125	154
27 k l			
1	0	125	110
1	1	532	485
1	2	65	16-
1	3	142	115
1	4	343	312-
1	5	195	185-
1	6	55	82
1	7	111	159-
1	8	25·	57-
1	9	349	367
1	10	11·	19-
28 k l			
0	0	96	107
2	0	333	330-
2	1	433	441
0	2	94	87
2	2	444	122
0	4	634	542-
0	6	493	469-
0	8	538	553
29 k l			
1	0	282	354
1	1	963	941
1	2	474	457
1	3	402	387
1	4	210	278

notably twisted and distorted. It shares no edge with silicon tetrahedra; it shares one edge [$\overline{\mathrm{O(7)O(9)}}$ = 2·61 Å] with the beryllium tetrahedron, a second [$\overline{\mathrm{O(3)O(4)}}$ = 2·61 Å] with the aluminum tetrahedron, and a third [$\overline{\mathrm{O(8)O(9)}}$ = 3·05 Å] with another calcium polyhedron. Moreover it shares only corners [O(2), O(3), O(4), O(7) and O(9)] with five silicon tetrahedra, one [O(8)] with a beryllium tetrahedron and one [O(2)] with a calcium polyhedron.

Although bavenite is a calcium silicate, it does not belong to the class of silicates named second 'chapter' by Belov (1961). In fact the calcium coordination polyhedron is not an octahedron, and the lengths of its edges vary over a large interval, approximately between 2·5 and 4·5 Å. Occasionally 'diortho groups' ($Si_2O_7^{6-}$) adapt themselves to the larger edges, but in a random way. Here the flexibility of the silicate chains, claimed by Belov, is not sufficient to allow calcium to assume a regular octahedral coordination.

Table 4. *Interatomic distances* (Å), *angles* (°) *and their standard deviations* (*in brackets*)

The distances and angles preceded by an asterisk occur twice

Atoms	Bond length	Mean
T(1)O(1)	* 1·650(5)	
T(1)O(9)	* 1·603(5)	1·626
T(2)O(7)	* 1·606(7)	
T(2)O(8)	1·679(14)	
T(2)O(9)	1·673(11)	1·641
T(3)O(1)	1·684(4)	
T(3)O(3)	1·599(5)	
T(3)O(2)	* 1·549(5)	1·608
T(4)O(3)	* 1·725(4)	
T(4)O(4)	* 1·732(6)	1·729
T(5)O(4)	* 1·621(5)	
T(5)O(5)	* 1·604(4)	1·613
T(6)O(6)	1·608(6)	
T(6)O(6′)	1·638(6)	
T(6)O(5)	1·616(4)	
T(6)O(7)	1·593(5)	1·614
Ca O(7)	2·343(6)	
Ca O(2)	2·344(3)	
Ca O(8)	2·410(4)	
Ca O(3)	2·448(6)	
Ca O(9)	2·463(4)	
Ca O(4)	2·507(4)	
Ca O(1)	2·639(4)	
Ca O(6)	3·816(6)	
Ca O(5)	3·882(6)	

Atoms	Angle	Mean
O(1)*T*(1)O(9)	** 109·1(1)	
O(1)*T*(1)O(1′)	103·9(5)	
O(9)*T*(1)O(9′)	115·8(6)	109·4
O(7)*T*(2)O(8)	* 110·1(5)	
O(7)*T*(2)O(9)	* 105·7(5)	
O(8)*T*(2)O(9)	109·4(6)	
O(7)*T*(2)O(7′)	115·6(1·4)	109·4
O(1)*T*(3)O(3)	* 100·9(2)	
O(3)*T*(3)O(3′)	112·1(6)	
O(2)*T*(3)O(3)	* 115·8(3)	
O(1)*T*(3)O(2)	109·1(3)	109·1
O(3)*T*(4)O(4)	* 98·2(2)	
O(4)*T*(4)O(4′)	123·1(5)	
O(3)*T*(4)O(3′)	117·5(5)	
O(3)*T*(4)O(4′)	* 110·6(3)	109·7
O(4)*T*(5)O(4′)	112·2(6)	
O(5)*T*(5)O(5′)	114·0(5)	
O(4)*T*(5)O(5)	* 107·1(2)	
O(4)*T*(5)O(5′)	* 108·4(2)	109·5
O(5)*T*(6)O(6)	108·3(3)	
O(5)*T*(6)O(6′)	107·6(3)	
O(5)*T*(6)O(7)	111·6(3)	
O(6)*T*(6)O(6′)	107·3(6)	
O(6)*T*(6)O(7)	109·3(3)	
O(6)*T*(6)O(7′)	112·6(3)	109·5
T(1)O(1)*T*(3)	116·3(3)	
Ca O(2) Ca′	112·7(4)	
Ca O(2) *T*(3)	* 105·4(3)	
T(3)O(3)*T*(4)	149·6(3)	
Ca O(3)*T*(4)	100·2(3)	
Ca O(3)*T*(3)	104·0(2)	
T(4)O(4)*T*(5)	130·2(2)	
T(4)O(4)Ca	97·8(2)	
T(5)O(4)Ca	130·5(3)	
T(5)O(5)*T*(6)	141·2(4)	
T(6)O(6)*T*(6′)	135·6(6)	
T(6)O(7)*T*(2)	132·8(5)	
Ca O(7)*T*(2)	96·5(4)	
Ca O(7)*T*(6)	130·6(3)	
Ca O(8)Ca′	103·5(5)	
Ca O(8)*T*(2)	* 121·8(2)	
Ca O(9)Ca′	100·4(4)	
Ca O(9)*T*(2)	* 90·4(3)	
Ca O(9)*T*(1)	* 121·3(2)	
T(1)O(9)*T*(2)	125·3(6)	

Balance of the electrostatic valences

In accordance with the suggestions made above, Table 5 shows a balance of electrostatic valences constructed on the following assumptions:

(i) The coordination number of the calcium ion is six.

(ii) The hydrogen atom is linked to O(8).

Table 5. *Balance of electrostatic valences*

	Ca	H	Si	Be	Al	Total
O(1)			2×1			2
O(2)	$2\times\frac{1}{3}$		1			$2-\frac{1}{3}$
O(3)	$\frac{1}{3}$		1		$\frac{3}{4}$	$2+\frac{1}{12}$
O(4)	$\frac{1}{3}$		1		$\frac{3}{4}$	$2+\frac{1}{12}$
O(5)			2×1			2
O(6)			2×1			2
O(7)	$\frac{1}{3}$		1	$\frac{1}{2}$		$2-\frac{1}{6}$
O(8)	$2\times\frac{1}{3}$	1		$\frac{1}{2}$		$2+\frac{1}{6}$
O(9)	$2\times\frac{1}{3}$		1	$\frac{1}{2}$		$2+\frac{1}{6}$

Although the balance is hardly satisfactory for O(2), the Si–O and Ca–O distances for this atom are found to be by far the shortest ones in this structure; so the figure quoted in Table 5 for O(2) should be increased, and this results in a satisfactory balance for this atom. Also the Ca–O(7) distance is very short, therefore the figure quoted for O(7) should be increased too.

Positions of the hydrogen atoms

The hypothesis has been put forward that one hydroxyl is linked to each beryllium atom, on the basis of the chemical formula of bavenite; the oxygen involved is assumed to be O(8) because it corresponds to a break in the tetrahedral framework. The satisfactory balance of charges around O(8) is founded on this statement and affords a very important confirmation of the hypothesis; otherwise the sum of charges around O(8) would have been inadmissibly low $(1+\frac{1}{6})$.

Some further evidence for this statement can be derived from the final three-dimensional difference synthesis, computed in the structure voids that may be occupied by the hydrogen atoms. This synthesis shows a maximum – the highest – with coordinates $(x/a, y/b, z/c) = (0{\cdot}100, 0{\cdot}267, 0{\cdot}250)$, corresponding to an O(8)–H distance of about 1·2 Å and to an angle Be–O(8)–H of about 112°.

Description of the structure

Bavenite displays a type of framework unknown till now. For descriptive purpose it is convenient to include Al and Be in the system of linked tetrahedra; in this way the crystal structure approaches without reaching the rank of a tetrahedral framework. In fact the ratio between the number of tetrahedral cations and that of oxygen anions is 13:28; only two out of fourteen oxygen atoms interrupt the three-dimensional linking of tetrahedra: they are O(2) and O(8) and belong to Be and $T(3)$ respectively (the first of them is linked to a hydrogen atom). The tetrahedra that break the framework are disposed in a comparable way in the structure; both have the not-linking T–O bond nearly parallel to **b** and lying on a mirror plane; as a difference Be–O(8) and $T(3)$–O(2) have opposite directions [Fig. 3(*f*)].

Perhaps the main feature of this crystal structure is a fourfold chain of tetrahedra developing along the *b* axis and built up by four pyroxene-like chains connected circularly between themselves. The projection of the fourfold chain along **b**, that surrounds the point of coordinates $(\frac{1}{4}, \frac{1}{2})$ [Fig. 3(*a*)] displays circularly: chain I, chain II, chain I′, chain II′, where I and II denote equivalent chains; I and I′ are related by a diad axis, II and II′ by a *b*-glide plane. Chain I is built up from equivalent tetrahedra: $\cdots -T(6)-O(6)-T(6)- \cdots$, that are repeated by the *b*-glide plane; it can be seen clearly in Fig. 3(*b*) (*d*) and (*e*). Chain II is composed of the –Al–O(4)–$T(5)$– unit that repeats for simple translation along **b**; it appears in Fig. 3(*b*), and also in Fig. 3(*d*) behind chain I; in this chain the cations are all disposed on the diads. Within the fourfold chain a ring of six silicon atoms arises; it can be seen in Fig. 3(*a*). The unit translation along **b**, 5·005 Å, is related to the existence of these chains.

Two different fourfold chains are connected along **c** through two beryllium tetrahedra as bridges, forming a system $S(1)$ of six-membered rings running zigzag along **b**. Moreover two different fourfold chains are connected along **a** through two $T(3)$ tetrahedra as bridges, forming a system of rings $S(2)$ of alternately four and eight tetrahedra running parallel to **b**. Each one of these systems is cut in the middle by a mirror plane parallel to **b**; the mirror planes are perpendicular and cross in $T(1)$.

These two systems of rings, $S(1)$ and $S(2)$, are connected through rings of six non-equivalent tetrahedra, shown in Fig. 3(*f*); the calcium atoms occupy the channels formed by them along **b**. Four calcium polyhedra are interconnected, related by the mirror planes crossing at $T(1)$; no connections exist between calcium polyhedra along **b**.

In this crystal structure there are no empty channels and therefore bavenite has no zeolitic character; its density is comparatively high, over 2·71 g.cm^{-3}.

Cleavage

The {001} cleavage is very good and can readily be explained from consideration of Fig. 3(*a*). A plane $z/c \simeq \frac{1}{5}$ [approximately between the *z* coordinates of O(7) and O(8)] cuts a minimum number of Si–O–Si bonds, no Ca–O bonds and many Be–O bonds. The good {100} cleavage can be explained in a similar way.

Diadochy between the tetrahedral cations

The numbers of beryllium and aluminum atoms in the chemical formula of the specimen available to us are nearly integers – with a small excess of beryllium and a corresponding defect of aluminum; moreover, according to this structure analysis, Al and Be occupy independent positions in the unit cell. Thus a conclusive discussion of the Be–Al diadochy is not possible here. The excess of beryllium can enter the position

$T(4)$: some evidence arises from the short average Al–O distance. The specimens richer in beryllium have about one half of the aluminum replaced by beryllium; this substitution does not result in a variation of the electrostatic field around the oxygen atoms involved, O(3) and O(4), only if the hydrogen that accompanies beryllium distributes itself statistically between them. There is also much room around O(2) suitable for occupancy by hydrogen, without any need of a statistical distribution among more than one position; this could be a likely way because in many respects O(2) and O(8), or $T(3)$ and Be play similar roles in the structure, as pointed out above in this discussion. In this case the beryllium to aluminum substitution would result in a clear improvement of the sum of the electrostatic valences around O(2) quoted in Table 5, because the hydrogen that accompanies the beryllium excess would add its contribution to the latter sum. An increase of the distances $T(3)$–O(2) and Ca–O(2) parallel to the increase of the beryllium to aluminum substitution would strengthen this hypothesis, as an evidence that the shortness of these distances is less and less necessary to obtain the balance of the electrostatic valences around O(2).

There is no clear evidence to choose between these hypotheses; the diadochy could be even more complicated and involve also the silicon atoms: for example, diadochy between $T(1)$ and Al cannot be excluded to a small extent, owing to the long average $T(1)$–O distance and to the short Al–O one. However these open questions have been discussed here to point out that a comparison of the structure of this bavenite with that of a beryllium-rich one would be of interest in order to understand the details of diadochy between the tetrahedrally coordinated cations.

Chemical formula

The up-to-date more reasonable chemical formula of bavenite appears to be:

$$\mathrm{Ca_4(BeOH)_{2+x}Al_{2-x}Si_9O_{26-x}}, \quad \text{where } 0\cdot10 \le x \le 0\cdot84\,.$$

We wish to thank Professor F. Sgarlata who kindly made available to us his program for three-dimensional refinement by the least-squares method.

References

AHMED, F. R. & CRUICKSHANK, D. W. J. (1953). *Acta Cryst.* **6**, 385.

BELOV, N. V. (1961). *Crystal Chemistry of Large-Cation Silicates* (English translation), p. 3. New York: Consultants Bureau (1964). 3.

BERRY, L. G. (1963). *Amer. Min.* **48**, 1166.

CRUICKSHANK, D. W. J. (1949). *Acta Cryst.* **2**, 65, 154.

DARLOW, S. F. (1960). *Acta Cryst.* **13**, 683.

HAMILTON, W. C. (1957). *Acta Cryst.* **10**, 629.

MOORE, F. H. (1963). *Acta Cryst.* **16**, 1169.

SAKURAI, T. (1962). *Acta Cryst.* **15**, 443.

SMITH, D. K. (1959). *Acta Cryst.* **12**, 479.

Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

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Crystal data for (−)-*threo*-12,13-dihydroxyoleic acid.

By DAVID A. LUTZ and WILLIAM E. SCOTT, *Eastern Utilization Research and Development Division, Agricultural Research Service, U.S. Department of Agriculture, Philadelphia, Pa.* 19118, *U.S.A.*

(*Received* 20 *August* 1965)

The present study was undertaken to obtain crystal data on (-)-*threo*-12,13-dihydroxyoleic acid, $C_{18}H_{34}O_4$, which was prepared by acetolysis of the seed oil of *Vernonia anthelmintica* (L.) Willd. (Scott, Krewson & Riemenschneider, 1962). The compound was further purified [as evidenced by chemical analysis (C 68·5, H 10·8 %) and melting point (63–63·5 °C)] and single crystals were produced by a series of slow crystallizations from acetone at room temperature. Cell constants were determined from various oscillation and Weissenberg photographs, using Cu $K\alpha$ radiation (λ = 1·5418 Å). The density was measured by flotation. The space group was determined from systematic extinctions ($h00$, $0k0$ and $00l$ absent for h, k or l odd). The crystal data are as follows: $a = 5{\cdot}05 \pm 0{\cdot}01$, $b = 8{\cdot}51 \pm 0{\cdot}02$, $c = 44{\cdot}66 \pm 0{\cdot}05$ Å, $U = 1920$ Å^3, $z = 4$, $D_x = 1{\cdot}088$ g.cm^{-3}, $D_m = 1{\cdot}085$ g.cm^{-3}; space group, $P2_12_12_1$.

No further work on this compound is contemplated at present.

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References

SCOTT, W. E., KREWSON, C. F. & RIEMENSCHNEIDER, R. W. (1962), *Chem. and Ind.*, 2038.