The Structure of Euclase $HBeAlSiO_5$.

By

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(With 2 figures.)

Abstract.

From rotation and oscillation photographs made with a small splinter of Euclase the unit cell and space group have been determined. $a = 4.62$ Å, $b = 14.24$ Å, $c = 4.75$ Å, $\beta = 79° 44'$. The space group is C_{2h}^5 with glide along "*c*", and there are 4 molecules $HBeAlSiO_5$ per unit cell. A structure has been deduced by the usual cut and try methods. Each *Al* is octahedrally surrounded by 5 oxygens and one hydroxyl, each *Si* is tetrahedrally surrounded by 4 oxygens, and each *Be* is tetrahedrally surrounded by 3 oxygens and one hydroxyl. The Pauling rule is obeyed exactly. Quantitative measurements of the $0k0$ spectra are in good agreement with structure factors calculated from the structure. Coordinates are given for all the atoms, the "*b*" coordinates have been rather carefully determined, the "*a*" and "*c*" coordinates are only approximate.

Introduction.

Euclase $BeAlSiO_4(OH)$ is a member of the group of silicates commonly listed as the Datolite Group. From previous work on Euclase it seemed that this substance was the simplest member of the Datolite group, and therefore the most suitable material with which to begin an attack upon this group of minerals. The previously reported space group determination has turned out however to be wrong. The space group of Euclase is C_{2h}^5, a space group which is of but very little direct assistance in determining the atomic arrangement.

It has turned out to be impossible to derive the structure by any unique straight-forward method. The structure which is given below has been found by the usual cut and try methods, making use of all the known empirical laws of interatomic distance and bonding. In the direction of the "*b*" axis, the structure presents a rather simple aspect and the coordinates in this direction have been determined quite accurately. A precise determination of the other two coordinates would involve such a long tedious cut and try process that it did not seem worth the labor involved. The "a" and "c" coordinates which we have given here are accordingly only approximate.

Unit Cell and Space Group.

Rotation photographs were made about the three principal axes using M_0Ka radiation ($\lambda = .710$ Å). The sample used was a splinter from a crystal from Minas Geraes, Brazil. From the layer line distances the axil lengths were determined as follows:

$$a = 4.62\ \text{Å}$$
$$b = 14.24\ \text{Å} \qquad \beta = 79^\circ\, 44'\ ^{1})\text{.}$$
$$c = 4.75\ \text{Å}$$

These values are in good agreement with ones previously published²).

Using a density of 3.1 as given by Dana the number of molecules in the unit cell is calculated in the usual way

$$n = \frac{VN\varrho}{M} = \frac{4.62 \times 4.75 \times 14.24 \sin 79^\circ 44' \times 0.606 \times 3.1}{145} = 3.97.$$

There are accordingly 4 molecules $HBeAlSiO_5$ per unit cell.

Complete sets of 16° oscillation photographs were taken about the b and c axes. Reflexions of the type $0k0$ were observed only for k even and of the type $h0l$ only for l even. A considerable number of reflexions of each type were observed and there was ample opportunity for odd order reflexions to have occurred³).

The space group of Euclase is accordingly C_{2h}^5 rather than C_{2h}^2 as previously reported.

The symmetry elements of the space group will comprise symmetry centers, screw axes parallel to b, and a glide plane with glide in the direction of "c". Four assymetric atoms are required for the general position and hence all the atoms in Euclase may occupy general positions. The combination of a screw axis and a glide plane is a combination which is of very little help in fixing the positions of the atoms and it is for this reason that the structure which wo propose has been obtained solely by the cut and try method.

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1) E. S. Dana, "Textbook of Mineralogy".

2) B. Gossner and F. Mussgnug, Z. Krist. **70**, 171. 1929.

3) The reflexions $h0l$ with l odd which were recorded by Gossner were evidently reflexions of the type $h1l$. With such a long "b" axis these two types of reflexion $h0l$ and $h1l$ are easily confused unless the oscillation is made about the b axis.

Quantitative Measurements.

Measurements of the integrated intensities for the first twelve orders of the $0k0$ plane were made with a Bragg ionization spectrometer using M_0Ka radiation. The measurements were made by the transmission method using a thin slip of the crystal 0.121 cms. thick and cut so that the $0k0$ planes were normal to the plane of the slip. The integrated intensity ϱ is given by the relation[1])

$$= \left(N \frac{e^2}{m c^2} F\right)^2 \lambda^3 \frac{1 + \cos^2 2\theta}{2 \sin 2\theta} \mu t \sec \theta \, e^{-\mu t \sec \theta}$$

where N is the number of unit cells per unit volume.

F is the structure factor per unit cell.
t is the thickness of the crystal slip.
μ is the linear absorption coefficient.
e, m, c and λ have the usual meaning.

Comparison was made against the 600 reflexion from rock salt for which ϱ was taken to be 21.7×10^{-6}. For μ a value of 8.22 cm was used, which was an average of the value obtained by direct measurement and by calculation from the tables of atomic absorption coefficients. From the measured values of ϱ the structure factors F are readily calculated, and the values so obtained are listed in the fourth column of Table I.

Table I.

Comparison of Calculated and Measured F for $0k0$ Planes.

$0k0$	$\sin \theta$	$\varrho \times 10^6$ (meas.)	$\pm F$ (meas.)	F (calc.)
020	.0499	256	46.4	+ 44
040	.0998	39.4	24.4	— 24
060	.150	15.0	18.6	+ 10
080	.199	52.1	40.5	— 53
0100	.249	—	—	— 5
0120	.299	13.7	26.0	— 32
0140	.349	10.1	25.2	— 30
0160	.399	1.8	11.6	+ 13
0180	.449	7.0	24.8	+ 17
0200	.499	6.2	24.8	+ 24
0220	.549	—	—	— 1
0240	.598	—	—	+ 16

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[1]) W. L. Bragg and J. West, Z. Krist. **69**, 123. 1928.

Proposed Structure.

The main features of the proposed structure are best seen from the schematic representation in Fig. 1b. Each aluminum is octahedrally surrounded by 5 oxygens and one hydroxyl, each silicon is tetrahedrally surrounded by 4 oxygens, and each *Be* is tetrahedrally surrounded by 3 oxygens and one hydroxyl. The Pauling rule of valence bonds is satisfied exactly for the four oxygens and the hydroxyl.

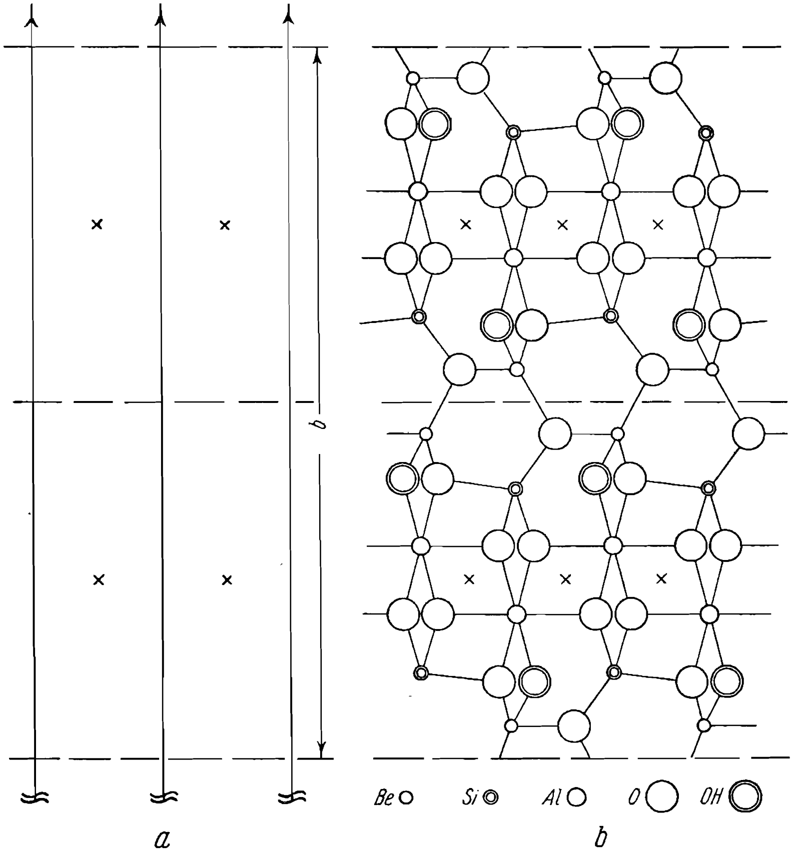

Fig. 1. a. Symmetry elements of C_{2h}^5.
b. Structure of Euclase projected upon (*a*, *b*) plane.

From the schematic structure represented in Fig 1b, approximate values for the θ_2 coordinates are readily assigned. By comparison of the calculated and observed structure factors slight improvements in the coordinates are then made. The calculated values of structure factors listed in column 5 of Table I are calculated from the θ_2 coordinates obtained in this way. The agreement between calculated and measured F is very satisfactory.

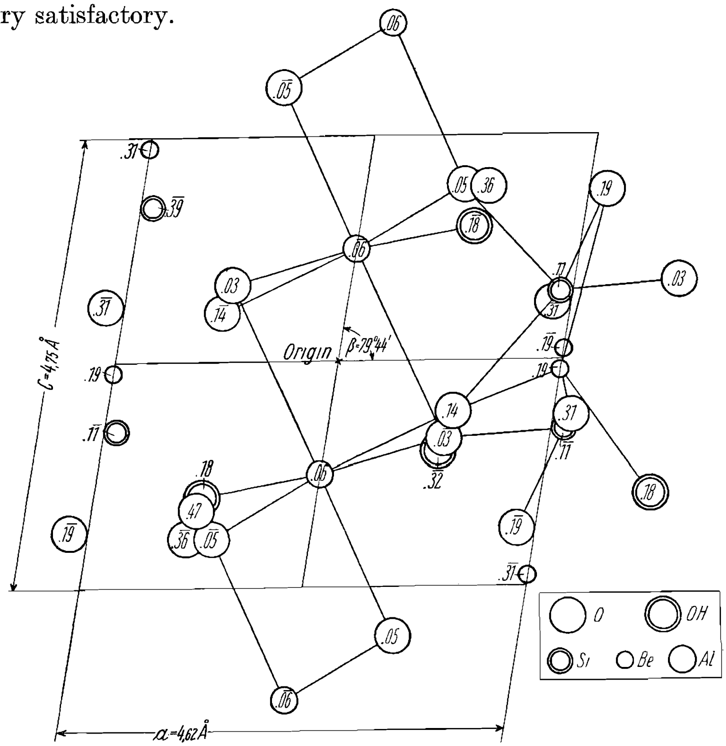

Fig. 2. Structure of Euclase projected upon (a, c) plane.

In Fig. 2 is shown a projection of the structure upon the a c plane. As stated before, the θ_1 und θ_3 coordinates must be considered as only approximate. In Table II are listed the coordinates of the atoms expressed both in degrees and in decimal parts of the axial lengths.

Table II.

Atomic Coordinates. (Measured from a symmetry center as origin.)

	θ_1	θ_2	θ_3	X	Y	Z
Be	180	— 70	+ 8	.50	— .20	.02
A	10	— 20	+ 90	.03	— .06	.25
Si	170	+ 35	+ 55	.47	.10	.15
O_1	80	+ 18	+ 140	.22	.05	.39
O_2	95	— 11	— 62	.26	— .03	— .17
O_3	195	+ 69	+ 135	.54	.19	.37
O_4	— 100	— 52	+ 40	— .28	— .15	.11
OH	+ 80	— 60	+ 110	.22	— .17	.31

Using the approximate θ_1 und θ_3 coordinates, calculated values of the intensity of $h00$ and $00l$ planes are in satisfactory qualitative agreement. While it has not been possible to deduce the proposed structure as a unique solution, it is nevertheless true that the proposed structure is in complete agreement with the empirical rules for silicate structures and with the available data.

Particulary interesting is the ready explanation which the structure gives for the perfect cleavage parallel to (010). As seen in Fig. 1b, the structure is held together across the glide plane only by a few weak *Be—O* bonds.

During the course of the work we plotted out the Fourier distribution parallel to the "*b*" axis by taking the 8 strongest $0k0$ amplitudes and plotting out the 128 possible combinations of signs. It was hoped that impossible concentrations of scattering matter, or large negative densities would occur on enough of the curves to rule out all but few. Actually it was found that out of the 128 curves there remained about 40 which seemed to represent reasonable distributions of scattering matter. Altho it was impossible to pick out any one of these 40 as representing the correct structure, nevertheless it was noticed that for the 40 remaining curves the sign of any one harmonic was either positive or negative in the majority of the curves. From statistical considerations of this sort it was possible to deduce the signs of three or four of the strongest harmonics. The structure itself however could not be definitely deduced from the curves, and our attempt to derive the structure directly from the Fourier curves was unsuccessful.

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