The crystal structures and crystal chemistry of väyrynenite, (Mn, Fe) Be (PO$_4$) (OH), and euclase, AlBe (SiO$_4$) (OH)*

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With 2 figures

Auszug

Die Bestimmung und Verfeinerung der Kristallstrukturen von Väyrinenit und Euklas zeigen, daß diese Strukturen ähnlich, aber nicht identisch sind. Väyrinenit weist Ketten von BeO$_2$(OH)$_2$- und PO$_4$-Tetraedern auf, die durch Mn-O- und Wasserstoffbindungen verknüpft sind; Euklas enthält Ketten von BeO$_3$(OH)- und SiO$_4$-Tetraedern, zusammengehalten durch Al-O-Bindungen. Die Verschiedenheit beider Strukturen beruht hauptsächlich darauf, daß in der einen Struktur, die Mn und P enthält, die elektrostatischen Ladungen anders verteilt sind als in der Struktur mit Al und Si.

Abstract

Determination and refinement of the crystal structures of väyrynenite and euclase show that these minerals have related, but not identical, structures. Väyrynenite contains chains of BeO$_2$(OH)$_2$ and PO$_4$ tetrahedra linked by Mn-O and hydrogen bonds; euclase contains chains of BeO$_3$(OH) and SiO$_4$ tetrahedra linked by Al-O bonds. The differences between the two structures are due principally to the difference in electrostatic charge distribution between a structure containing Mn and P and a structure containing Al and Si.

During mineralogical investigation of the rare mineral väyrynenite, (Mn^{+2}, Fe^{+2}) Be(PO$_4$)(OH), a search of *Crystal data* (DONNAY and NOWACKI, 1954) revealed that väyrynenite and euclase, AlBe(SiO$_4$)(OH), have very close c/b ratios and relatively close a/b ratios. This observation, coupled with the fact that both minerals have the same chemical-formula type, AB (XO$_4$) Z, similar physical properties, and perfect cleavage parallel to (010), suggested that the two minerals might be isotypic. Although the x-ray powder-diffraction patterns of the two minerals differ considerably, precession photographs of their

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*hk*0, *h*0*l*, and 0*kl* nets are similar (MROSE and VON KNORRING, 1959, Fig. 3). In order to elucidate the relationship of these minerals, we have determined the crystal structure of väyrynenite and re-examined and refined the crystal structure of euclase, originally determined by BISCOE and WARREN (1933).

It is a pleasure for us to acknowledge the cooperation of Dr. GEORGE SWITZER of the U. S. National Museum, who made available the crystal of euclase used in our work. Special thanks are due to our colleague, HOWARD T. EVANS, JR., who gave encouragement, valuable advice, and helpful discussion throughout this study and made the final drawings for Figs. 1 and 2.

Experimental work
Crystal description and crystallographic data

The crystal of väyrynenite used for the structure determination is from the Viitaniemi pegmatite in the parish of Eräjärvi in central Finland (MROSE and VON KNORRING, 1959); it is euhedral (about 0.25 by 0.25 by 0.30 mm), translucent, pale Congo pink according to Ridgway's color standards and nomenclature (1912), prismatic elongated along [001] with $m\{110\}$ dominant over $b\{010\}$ and $c\{001\}$. Data for the redetermination and refinement of the structure of euclase were obtained from a small $\{010\}$ cleavage fragment (about 0.25 by 0.25 by

Table 1. *Crystallographic data for väyrynenite and euclase from* MROSE and VON KNORRING (1959)

	Väyrynenite	Euclase
Cell data		
a	5.411 $\pm$ 0.005 Å	4.763 $\pm$ 0.005 Å
b	14.49 $\pm$ 0.02	14.29 $\pm$ 0.02
c	4.730 $\pm$ 0.005	4.618 $\pm$ 0.005
β	102°45′ $\pm$ 05′	100°15′ $\pm$ 05′
$a:b:c$	0.373:1:0.326	0.333:1:0.323
Space group	$P2_1/a—C_{2h}^5$	$P2_1/a—C_{2h}^5$
Cell contents	$4[(Mn,Fe)Be(PO_4)(OH)]$	$4[AlBe(SiO_4)(OH)]$
Volume	361.7 Å^3	309.3 Å^3
Density, g · cm^{-3}		
(calc.)	3.23 (for Mn:Fe = 85:15)	3.115
(obs.)	3.215 $\pm$ 0.005 (microbalance)	3.095 $\pm$ 0.005 (microbalance)
	3.22 (suspension method)	

0.25 mm), cleaved from a pale emerald-green euclase crystal from Villa Rica, Minas Gerais, Brazil (USNM R3775). Single-crystal x-ray data for both minerals, as well as indexed powder-diffraction data, were reported by MROSE and VON KNORRING (1959); the single-crystal data are repeated in Table 1 for convenience.

Intensity data

Triple-film Weissenberg patterns using Mo/Zr and Cu/Ni radiations were taken of the $hk0$ and $0kl$ zones of väyrynenite and euclase. The films, interleaved with 0.0005 inch Ni foil, were given long and short exposures of 72 hours and 9 hours, respectively, with molybdenum radiation at 50 kV and 20 mA. In addition, exposures were made of both minerals with copper radiation in order to obtain intensity data for reflections with small Bragg angles.

For each mineral the intensities were estimated visually by direct comparison with a standard calibrated spot strip, prepared in the Weissenberg camera using a selected reflection from the respective $hk0$ pattern. Intensity data were collected to the value $(\sin\theta)/\lambda = 1.0$ Å^{-1} for the $hk0$ zone of väyrynenite, and to the value $(\sin\theta)/\lambda = 1.4$ Å^{-1} for the $hk0$ zone of euclase and the $0kl$ zones of both minerals. Intensity data were estimated for 187 non-equivalent $hk0$ and 277 non-equivalent $0kl$ reflections of väyrynenite, and for 262 non-equivalent $hk0$ reflections and 204 non-equivalent $0kl$ reflections of euclase. The estimated intensities were converted to F^2_{hkl} values by applying Lorentz and polarization corrections, calculated with a digital computer for each reciprocal-lattice point as a function of its cylindrical coordinates. The intensity data for each zone, read from the several films, were placed on the same relative scale by the use of appropriate film factors, based on a comparison of intensity readings of equivalent reflections appearing on more than one film. The multiple-film technique gave a range in scaled F^2_{hkl} of approximately 1 to 1000 for both minerals.

Because small and nearly equant crystals were used for collecting the intensity data, absorption errors were minimized and no corrections were attempted.

Other considerations

During the course of the determination and refinement of the crystal structures, described in the following sections, all Fourier syntheses were carried out on a Burroughs 205 computer using a pro-

gram devised by H. T. EVANS, JR. (1959). Structure-factor and least-squares calculations, including the calculation of standard errors in the atomic parameters, were performed on the same computer with a program written by E. MONASTERSKI and D. E. APPLEMAN of the U. S. Geological Survey (written communication); the formulas and procedures followed are described in detail in CLARK and CHRIST (1959). During each structure-factor calculation, the overall isotropic temperature coefficient B and the scale factor relating observed and calculated structure factors were refined by a least-squares method. The following atomic scattering factors were used: Be^0, O^0, Al^{+3}, and Si^{+4} from BERGHIUS and others (1955); P^0 from *Internationale Tabellen* (1935); and Mn^0 from THOMAS and UMEDA (1957). The effect of 15 atom-percent substitution of Fe^{+2} for Mn^{+2} on the atomic scattering-factor curve is slight and has been neglected. Maxima on the Patterson and electron-density projections were calculated by the method of BOOTH (1948).

Determination and refinement of the structures

A. Väyrynenite

The determination of the structure of väyrynenite was begun by preparing a Patterson projection on the plane normal to [001]. The resulting Patterson function showed many well-resolved peaks; those associated with the Mn-Mn, P-P, and Mn-P vectors were identified, and the following x and y coordinates were assigned: Mn, $x = 0.250$ and $y = 0.439$; P, $x = 0.197$ and $y = 0.102$. Structure factors calculated on the basis of these two atoms gave a residual factor R of 0.39 where

$$R = \Sigma ||F_{obs}| - |F_{calc}||/\Sigma|F_{obs}|,$$

excluding terms for which $|F_{obs}| = 0$. An electron-density projection along [001] was then calculated, using those terms for which signs were determined by the contributions of the Mn and P atoms to the structure factors. All the atoms in the structure (except for the hydrogen) were well resolved and easily identified on this projection.

The x and y coordinates taken from the first electron-density map are given in Table 2, column 1. The trial structure derived from this map consists of chains of $BeO_2(OH)_2$ and PO_4 tetrahedra, held together by octahedrally coordinated Mn. The oxygen atom not bonded to

Table 2. *Atomic positional parameters, standard errors, and temperature coefficients for väyrynenite*

Para-meters		Stage of refinement[1]				Standard errors in atomic parameters (in cycles)[2]		Individual isotropic temperature coefficients B_j based on parameters of column (4)	
		(1)	(2)	(3)	(4) (final)	(5)		(6) hk0	(7) 0kl
Mn	x	0.250	0.249	0.248	0.248	ε_x	0.0004		
	y	.439	.439	.439	.4390	ε_y	.0001		
	z	.935	.939	.940	.940	ε_z	.0003	0.51	0.36
P	x	.194	.194	.195	.195	ε_x	.0006		
	y	.099	.102	.104	.1045	ε_y	.0002		
	z	.541	.542	.539	.539	ε_z	.0005	.23	.14
O_1	x	.388	.376	.366	.366	ε_x	.0019		
	y	.046	.042	.041	.0401	ε_y	.0006		
	z	.775	.760	.753	.753	ε_z	.0014	.59	.40
O_2	x	.471	.469	.463	.463	ε_x	.0016		
	y	.365	.367	.366	.3662	ε_y	.0006		
	z	.667	.651	.654	.654	ε_z	.0015	.39	.40
O_3	x	.354	.353	.346	.346	ε_x	.0017		
	y	.190	.190	.193	.1932	ε_y	.0006		
	z	.511	.513	.506	.506	ε_z	.0015	.46	.37
O_4	x	.115	.109	.106	.106	ε_x	.0019		
	y	.060	.059	.060	.0600	ε_y	.0006		
	z	.242	.246	.245	.245	ε_z	.0014	.59	.40
O_5 (OH)	x	.206	.210	.212	.212	ε_x	.0018		
	y	.276	.276	.276	.2765	ε_y	.0006		
	z	.964	.964	.968	.969	ε_z	.0013	.74	.34
Be	x	.442	.433	.431	.431	ε_x	.0032		
	y	.268	.268	.264	.2640	ε_y	.0012		
	z	.801	.803	.784	.783	ε_z	.0029	.65	.65
R	hk0	.256	.137	.095	.085				
	0kl	.160	.130	.106	.091				
B	hk0	1.00	.49	.46	.46				
	0kl	.44	.33	.33	.33				

[1] See text for description of stage of refinement.

[2] For method of calculation see CLARK and CHRIST (1959).

R The residual factor; ΔF omitted in calculation if $F_{obs} = 0$.

B The average isotropic temperature coefficient (in Å^2).

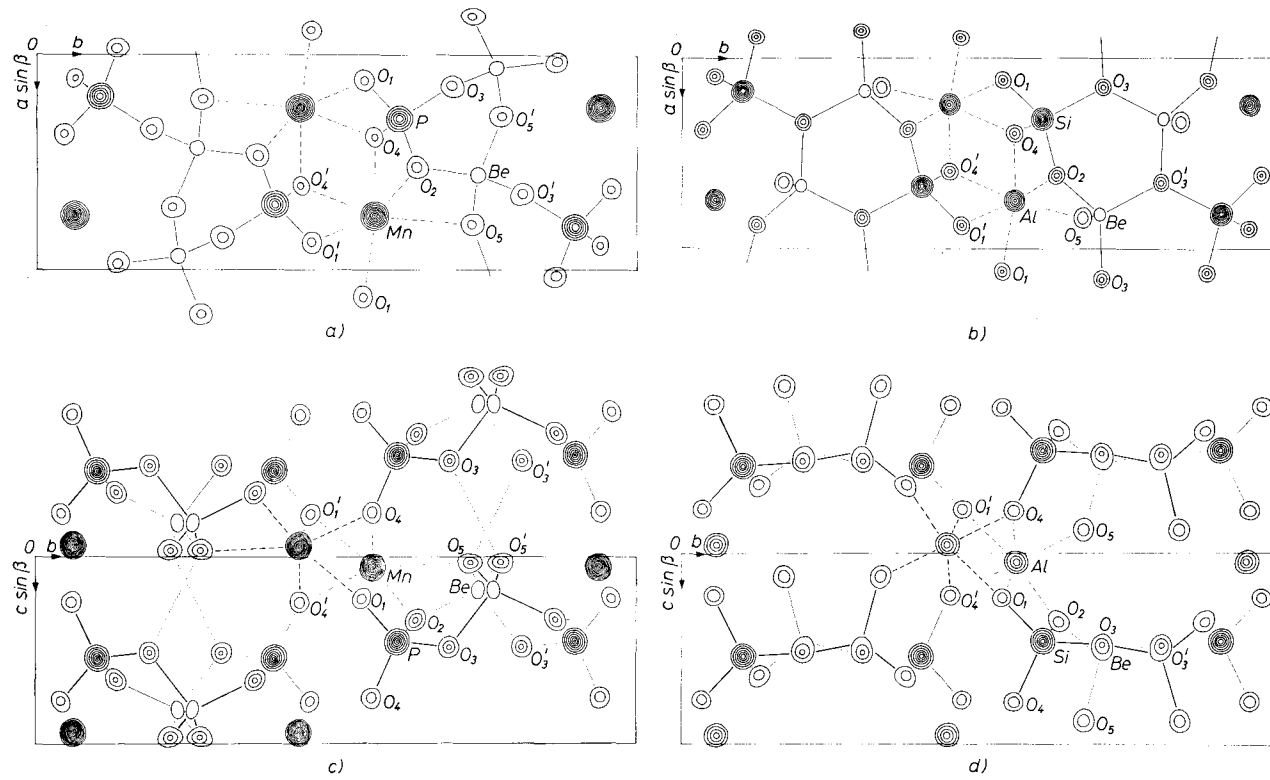ε_x The standard error in the positional parameter x of an atom.

Fig. 1. Electron-density projections of väyrynenite and euclase: contour interval $10\,e/\text{Å}^2$, zero contour omitted; (a) väyrynenite, projection along [001]; (b) euclase, projection along [001]; (c) väyrynenite, projection along [100]; (d) euclase, projection along [100]. Atoms are numbered to agree with Tables 7 and 8.

phosphorus is considered to be associated with the hydroxyl group. The R factor based on these coordinates is 0.26.

A second and third electron-density projection along [001] were then computed. In order to resolve the oxygen atoms more clearly, the third electron-density projection was calculated in the following manner. Structure factors consisting only of Mn and P contributions were calculated. A Fourier synthesis was then made using these values, subject to the same termination-of-series conditions imposed in the Fourier syntheses by the observed factors. The resulting electron-density distribution was subtracted point-by-point from the ordinary electron-density distribution, giving a projection essentially free from the effects of Mn and P. The second electron-density projection along [001], which was the final projection to include the contributions of the Mn and P atoms, is shown in Fig. 1a; it led to the x and y coordinates of Table 2, column 2.

Least-squares refinement of the $hk0$ zone was carried out in two stages: (1) five cycles, refining the positional parameters, an overall isotropic temperature factor, and the scale factor, yielded the x and y coordinates of Table 2, column 3; (2) eight cycles, fixing the scale factor and refining the positional parameters and individual isotropic temperature coefficients, yielded the x and y coordinates of Table 2, column 4. The final R factor for the $hk0$ zone is 0.085.

The z coordinates of the atoms in the väyrynenite structure were determined from the data of the $0kl$ zone, employing Patterson and electron-density projections along [100] and least-squares techniques, in a manner analogous to that of the $hk0$ refinement described above. The z coordinates of Table 2, columns 1 through 4, represent values at corresponding stages of refinement. The last complete electron-density projection along [100] is shown in Fig. 1c. A final projection, with the effects of Mn and P removed in the manner described above, yielded the z coordinates of Be and O in Table 2, column 2. Least-squares refinement was started with the y and z coordinates of Table 2, column 2; the final z coordinates after refinement with an overall temperature coefficient (five cycles) and individual isotropic temperature coefficients (six cycles) are shown in Table 2, columns 3 and 4, respectively. The y coordinates obtained from the two zones of data are virtually identical within the standard errors given in Table 2, column 5. Observed and calculated structure factors for the $hk0$ and $0kl$ zones of väyrynenite are listed in Table 3. The final residual factors are $R_{hk0} = 0.085$ and $R_{0kl} = 0.091$.

Table 3. *Comparison of observed and calculated structure factors for the hk*0 *and* 0*kl zones of väyrynenite*

h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c
2	0	0	90	-106	8	10	0	29	-31	4	23	0	10	11	0	20	2	15	13	0	9	5	16	17	0	8	8	–	9
4	0	0	40	39	9	10	0	11	-9	5	23	0	–	-3	0	21	2	13	-13	0	10	5	6	-7	0	9	8	–	0
6	0	0	24	-24	1	11	0	10	-9	6	23	0	–	-4	0	22	2	15	-13	0	11	5	–	5	0	10	8	8	8
8	0	0	12	12	2	11	0	–	3	0	24	0	35	-40	0	23	2	–	-4	0	12	5	6	3	0	11	8	11	11
10	0	0	12	-10	3	11	0	25	-27	1	24	0	13	9	0	24	2	35	-34	0	13	5	5	5	0	12	8	–	-4
1	1	0	20	28	4	11	0	16	15	2	24	0	30	32	0	25	2	–	3	0	14	5	5	3	0	13	8	10	10
2	1	0	7	5	5	11	0	20	18	3	24	0	7	-5	0	26	2	8	-9	0	15	5	16	17	0	14	8	8	-9
3	1	0	–	2	6	11	0	19	-18	4	24	0	19	-19	0	27	2	–	2	0	16	5	9	-12	0	15	8	8	-6
4	1	0	31	31	7	11	0	9	-8	5	24	0	–	4	0	28	2	–	1	0	17	5	20	22	0	16	8	9	-10
5	1	0	14	14	8	11	0	–	5	1	25	0	10	-10	0	29	2	10	10	0	18	5	–	-1	0	17	8	–	-2
6	1	0	14	-14	9	11	0	9	8	2	25	0	–	3	0	30	2	–	8	0	19	5	16	-13	0	18	8	16	-16
7	1	0	16	-14	0	12	0	34	-32	3	25	0	11	10	0	31	2	13	13	0	20	5	8	-10	0	19	8	10	-9
8	1	0	18	18	1	12	0	78	-87	4	25	0	–	-4	0	32	2	9	9	0	21	5	26	-23	0	20	8	–	-2
9	1	0	–	0	2	12	0	8	5	5	25	0	–	-2	0	33	2	–	2	0	22	5	–	6	0	21	8	–	5
10	1	0	–	0	3	12	0	54	56	0	26	0	18	-17	0	34	2	–	-3	0	23	5	16	-15	0	22	8	8	10
0	2	0	38	62	4	12	0	–	1	1	26	0	–	-2	0	35	2	10	-11	0	24	5	8	9	0	23	8	–	3
1	2	0	9	-4	5	12	0	30	-32	2	26	0	11	11	0	36	2	8	8	0	25	5	16	13	0	24	8	15	14
2	2	0	43	-42	6	12	0	–	-2	3	26	0	9	7	0	37	2	9	-11	0	26	5	–	4	0	25	8	–	-1
3	2	0	35	-36	7	12	0	–	2	4	26	0	19	-19	0	38	2	–	1	0	27	5	13	12	0	26	8	12	13
4	2	0	21	21	8	12	0	6	-6	1	27	0	8	-7	0	39	2	–	-1	0	28	5	–	0	0	27	8	–	-6
5	2	0	51	54	9	12	0	11	-9	2	27	0	11	13	0	0	3	8	7	0	29	5	6	5	0	28	8	–	-1
6	2	0	23	-24	1	13	0	8	9	3	27	0	–	0	0	1	3	46	-41	0	30	5	–	-5	0	29	8	–	0
7	2	0	23	-25	2	13	0	7	-7	0	28	0	–	1	0	2	3	14	11	0	31	5	–	-2	0	30	8	–	-5
8	2	0	25	23	3	13	0	5	3	1	28	0	12	-11	0	3	3	65	-68	0	32	5	–	-3	0	31	8	6	10
9	2	0	24	26	4	13	0	14	12	2	28	0	–	-2	0	4	3	13	12	0	33	5	–	-6	0	0	9	9	-10
10	2	0	10	-7	5	13	0	20	-21						0	5	3	44	-41	0	34	5	–	1	0	1	9	10	-10
1	3	0	22	-17	6	13	0	16	-15	0	2	0	40	62	0	6	3	5	-4	0	35	5	–	-2	0	2	9	–	-8
2	3	0	29	29	7	13	0	17	15	0	4	0	13	-12	0	7	3	4	4	0	36	5	5	-2	0	3	9	–	-1
3	3	0	12	-10	8	13	0	6	-8	0	6	0	83	-89	0	8	3	13	-10	0	37	5	4	-4	0	4	9	8	-9
4	3	0	18	18	9	13	0	6	-5	0	8	0	58	-64	0	9	3	32	31	0	0	6	17	-18	0	5	9	7	5
5	3	0	9	-9	0	14	0	–	5	0	10	0	32	-33	0	10	3	44	-43	0	1	6	–	-7	0	6	9	5	5
6	3	0	12	-11	1	14	0	18	-19	0	12	0	33	-32	0	11	3	25	26	0	2	6	27	-30	0	7	9	10	10
7	3	0	6	5	2	14	0	5	-3	0	14	0	–	6	0	12	3	8	-8	0	3	6	6	2	0	8	9	23	25
8	3	0	9	10	3	14	0	34	37	0	16	0	34	34	0	13	3	31	32	0	4	6	9	-9	0	9	9	–	-3
9	3	0	–	0	4	14	0	22	25	0	18	0	37	42	0	14	3	38	37	0	5	6	27	-29	0	10	9	11	12
10	3	0	9	7	5	14	0	29	-30	0	20	0	21	21	0	15	3	19	17	0	6	6	18	20	0	11	9	15	-16
0	4	0	16	-12	6	14	0	24	-26	0	22	0	7	-6	0	16	3	14	15	0	7	6	21	-22	0	12	9	–	1
1	4	0	32	32	7	14	0	10	9	0	24	0	40	-44	0	17	3	–	1	0	8	6	23	27	0	13	9	10	-8
2	4	0	12	-7	8	14	0	18	19	0	26	0	20	-19	0	18	3	–	6	0	9	6	7	-7	0	14	9	11	-12
3	4	0	66	-65	9	14	0	13	-11	0	28	0	–	1	0	19	3	30	-31	0	10	6	24	27	0	15	9	–	-1
4	4	0	13	-13	1	15	0	–	2	0	30	0	22	21	0	20	3	20	-18	0	11	6	28	31	0	16	9	17	-16
5	4	0	37	38	2	15	0	–	-2	0	32	0	14	13	0	21	3	39	-37	0	12	6	–	1	0	17	9	10	11
6	4	0	14	-14	3	15	0	18	19	0	34	0	–	-3	0	22	3	–	4	0	13	6	34	34	0	18	9	–	-6
7	4	0	27	-28	4	15	0	–	0	0	36	0	9	8	0	23	3	25	-24	0	14	6	–	-6	0	19	9	–	7
8	4	0	13	13	5	15	0	17	-17	0	38	0	–	-2	0	24	3	–	3	0	15	6	–	0	0	20	9	–	0
9	4	0	27	28	6	15	0	–	5	0	40	0	8	-8	0	25	3	8	9	0	16	6	11	-12	0	21	9	7	6
10	4	0	8	-7	7	15	0	10	9	0	0	1	15	23	0	26	3	12	-11	0	17	6	13	-14	0	22	9	7	7
1	5	0	45	-46	8	15	0	–	-5	0	1	1	35	-51	0	27	3	25	25	0	18	6	23	-19	0	23	9	–	-3
2	5	0	11	-10	9	15	0	–	4	0	2	1	32	42	0	28	3	–	-5	0	19	6	18	-18	0	24	9	9	8
3	5	0	48	47	0	16	0	33	33	0	3	1	35	-30	0	29	3	20	20	0	20	6	7	-5	0	25	9	7	3
4	5	0	7	-3	1	16	0	13	11	0	4	1	76	68	0	30	3	–	-1	0	21	6	–	3	0	26	9	–	3
5	5	0	29	-29	2	16	0	15	-17	0	5	1	17	-19	0	31	3	9	9	0	22	6	9	9	0	27	9	–	0
6	5	0	8	-9	3	16	0	–	1	0	6	1	50	-45	0	32	3	9	8	0	23	6	–	-4	0	28	9	5	7
7	5	0	10	7	4	16	0	21	21	0	7	1	–	1	0	33	3	–	-3	0	24	6	8	6	0	0	10	25	-27
8	5	0	–	4	5	16	0	8	-6	0	8	1	60	-62	0	34	3	8	8	0	25	6	–	-3	0	1	10	–	4
9	5	0	–	0	6	16	0	25	-26	0	9	1	21	-20	0	35	3	–	-2	0	26	6	11	9	0	2	10	17	-17
10	5	0	–	-6	7	16	0	10	11	0	10	1	78	-76	0	36	3	–	3	0	27	6	–	0	0	3	10	16	17
0	6	0	83	-89	8	16	0	22	23	0	11	1	–	-2	0	37	3	9	-10	0	28	6	–	0	0	4	10	–	7
1	6	0	52	51	1	17	0	12	9	0	12	1	7	0	0	38	3	5	-5	0	29	6	11	11	0	5	10	–	5
2	6	0	61	64	2	17	0	19	18	0	13	1	11	10	0	39	3	7	-9	0	30	6	–	-2	0	6	10	17	16
3	6	0	74	-84	3	17	0	8	-4	0	14	1	53	52	0	0	4	53	52	0	31	6	10	11	0	7	10	–	1
4	6	0	34	-34	4	17	0	20	-18	0	15	1	10	10	0	1	4	11	-11	0	32	6	7	-7	0	8	10	8	7
5	6	0	38	38	5	17	0	5	-8	0	16	1	29	31	0	2	4	6	5	0	33	6	–	1	0	9	10	9	-8
6	6	0	26	24	6	17	0	20	22	0	17	1	–	5	0	3	4	23	-24	0	34	6	11	-11	0	10	10	10	11
7	6	0	14	-12	7	17	0	–	2	0	18	1	25	27	0	4	4	9	9	0	35	6	7	-8	0	11	10	–	-3
8	6	0	5	-5	8	17	0	–	0	0	19	1	–	2	0	5	4	40	-41	0	0	7	28	-34	0	12	10	7	6
9	6	0	–	-5	0	18	0	38	39	0	20	1	18	-18	0	6	4	21	-21	0	1	7	24	-23	0	13	10	–	-2
10	6	0	–	-2	1	18	0	34	37	0	21	1	–	1	0	7	4	37	-37	0	2	7	9	-12	0	14	10	–	-3
1	7	0	13	12	2	18	0	39	-41	0	22	1	7	-8	0	8	4	17	-17	0	3	7	24	-24	0	15	10	9	-8
2	7	0	37	35	3	18	0	17	-18	0	23	1	7	-6	0	9	4	–	0	0	4	7	–	-1	0	16	10	–	-6
3	7	0	4	-2	4	18	0	24	24	0	24	1	8	-8	0	10	4	8	7	0	5	7	9	-11	0	17	10	–	0
4	7	0	41	-45	5	18	0	15	14	0	25	1	–	1	0	11	4	44	45	0	6	7	10	11	0	18	10	15	-15
5	7	0	16	15	6	18	0	19	-20	0	26	1	14	-13	0	12	4	7	-7	0	7	7	15	14	0	19	10	–	3
6	7	0	11	9	7	18	0	–	-2	0	27	1	–	4	0	13	4	51	55	0	8	7	23	23	0	20	10	–	-5
7	7	0	–	1	8	18	0	10	7	0	28	1	13	-11	0	14	4	16	-15	0	9	7	13	13	0	21	10	14	14
8	7	0	–	0	1	19	0	–	1	0	29	1	–	2	0	15	4	–	5	0	10	7	18	19	0	22	10	–	2
9	7	0	6	-2	2	19	0	17	-15	0	30	1	–	-3	0	16	4	–	-2	0	11	7	–	2	0	23	10	–	4
10	7	0	–	-2	3	19	0	23	-22	0	31	1	8	-7	0	17	4	21	-20	0	12	7	7	7	0	24	10	9	11
0	8	0	58	-63	4	19	0	5	4	0	32	1	20	17	0	18	4	14	14	0	13	7	9	7	0	0	11	6	-5
1	8	0	11	9	5	19	0	10	10	0	33	1	–	-5	0	19	4	27	-27	0	14	7	13	-13	0	1	11	–	0
2	8	0	53	58	6	19	0	–	3	0	34	1	21	21	0	20	4	12	12	0	15	7	7	6	0	2	11	–	0
3	8	0	16	-15	7	19	0	–	-4	0	35	1	–	1	0	21	4	5	-7	0	16	7	26	-25	0	3	11	9	11
4	8	0	18	-17	0	20	0	21	20	0	36	1	–	3	0	22	4	–	0	0	17	7	–	6	0	4	11	9	-10
5	8	0	–	2	1	20	0	19	21	0	37	1	–	0	0	23	4	8	-9	0	18	7	8	-5	0	5	11	–	6
6	8	0	31	32	2	20	0	15	-16	0	38	1	11	-12	0	24	4	13	-14	0	19	7	16	-14	0	6	11	7	0
7	8	0	14	14	3	20	0	24	-28	0	39	1	–	-2	0	25	4	–	-4	0	20	7	–	-3	0	7	11	14	9
8	8	0	36	-37	4	20	0	–	-2	0	40	1	7	-8	0	26	4	5	6	0	21	7	19	-18	0	8	11	–	13
9	8	0	8	-7	5	20	0	10	10	0	0	2	71	70	0	27	4	10	8	0	22	7	–	4	0	9	11	10	4
10	8	0	20	19	6	20	0	–	4	0	1	2	–	-2	0	28	4	–	1	0	23	7	16	-17	0	10	11	8	10
1	9	0	12	11	7	20	0	22	-20	0	2	2	15	-12	0	29	4	20	17	0	24	7	13	13	0	11	11	–	-9
2	9	0	17	16	1	21	0	–	2	0	3	2	10	-7	0	30	4	–	4	0	25	7	9	8	0	12	11	8	2
3	9	0	17	-17	2	21	0	18	-17	0	4	2	23	-19	0	31	4	17	16	0	26	7	9	9	0	13	11	10	-11
4	9	0	7	6	3	21	0	–	3	0	5	2	65	-64	0	32	4	–	2	0	27	7	14	15	0	14	11	–	-9
5	9	0	20	20	4	21	0	–	4	0	6	2	38	-37	0	33	4	–	0	0	28	7	7	6	0	15	11	9	-4
6	9	0	12	12	5	21	0	7	7	0	7	2	40	-33	0	34	4	–	-5	0	29	7	10	10	0	0	12	4	-3
7	9	0	–	-6	6	21	0	7	-7	0	8	2	29	-25	0	35	4	10	-10	0	30	7	6	-7	0	1	12	–	3
8	9	0	–	-2	7	21	0	10	-10	0	9	2	14	13	0	36	4	–	2	0	31	7	–	1	0	2	12	–	–
9	9	0	–	-5	0	22	0	11	-5	0	10	2	33	31	0	37	4	14	-16	0	32	7	7	-9	0	3	12	7	10
10	9	0	–	4	1	22	0	–	0	0	11	2	39	41	0	0	5	17	-19	0	33	7	–	-3	0	4	12	6	4
0	10	0	33	-33	2	22	0	16	16	0	12	2	–	1	0	1	5	30	-31	0	0	8	12	-14	0	5	12	7	9
1	10	0	23	-21	3	22	0	12	-13	0	13	2	28	30	0	2	5	11	-11	0	1	8	9	8	0	6	12	7	8
2	10	0	5	4	4	22	0	10	-9	0	14	2	–	2	0	3	5	33	-40	0	2	8	11	-14	0	7	12	5	5
3	10	0	36	37	5	22	0	19	20	0	15	2	7	7	0	4	5	13	13	0	3	8	10	12	0	8	12	6	-6
4	10	0	22	-21	6	22	0	10	10	0	16	2	11	11	0	5	5	37	-43	0	4	8	9	6	0	9	12	5	-6
5	10	0	11	-11	1	23	0	5	-4	0	17	2	4	-6	0	6	5	–	3	0	5	8	8	-10	0	10	12	6	-7
6	10	0	38	39	2	23	0	9	-8	0	18	2	30	28	0	7	5	6	2	0	6	8	16	18	0	11	12	5	-7
7	10	0	17	17	3	23	0	12	12	0	19	2	22	-22	0	8	5	12	15	0	7	8	11	-13					

B. Euclase

The crystal structure of euclase was derived by BISCOE and WARREN (1933) using trial-and-error methods. Because of the stated inaccuracy in the atomic parameters listed in their paper and the contradictory positions shown for beryllium, we decided to redetermine and refine the euclase structure for comparison with that of väyrynenite. Assuming the two minerals to be approximately isotypic, the

analysis was begun by calculating structure factors for the $0kl$ zone of euclase, using the y and z coordinates from the corresponding final complete electron-density projection of väyrynenite. Signs from these structure factors were then used to compute the first electron-density projection along [100], which resolved clearly all the atoms except for Be and the hydroxyl oxygen O_5. Two possible locations for each of these two atoms were indicated, one set corresponding to that in the väyrynenite structure and one set in new positions. The y and z coordinates of Table 4, column 2, include the Be and O_5 positions corresponding to väyrynenite; the R factor for these coordinates is 0.55. Subsequent refinement showed that the alternate positions for Be and O_5 were, in fact, the correct ones; the y and z parameters from the first electron-density projection along [100] (Fig.1d), yielding an R factor of 0.24, are given in Table 4, column 3.

A trial structure of euclase, derived from the electron-density projection along [100], consisted of chains of $BeO_3(OH)$ and SiO_4 tetrahedra, held together by octahedrally coordinated Al. The oxygen atom not bonded to silicon is considered to be associated with the hydroxyl group. Least-squares refinement was then carried out on the data of the $0kl$ zone; column 4 (Table 4) shows the y and z parameters obtained after five cycles of refinement with an overall temperature coefficient; and column 5 (Table 4) shows the final y and z parameters after twelve cycles of refinement including individual isotropic temperature coefficients.

The differences noted above between the väyrynenite and euclase structures led us to compute a Patterson projection along [001] before attempting refinement of the $hk0$ zone of euclase. Comparison of the two Patterson maps showed sufficient similarity to justify calculation of the electron-density projection of euclase along [001], using signs based on x and y coordinates of Al and Si from the Patterson projection, y coordinates for all remaining atoms from the $0kl$ refinement of euclase (Table 4, column 5), and x coordinates for the oxygen atoms from the final parameters for väyrynenite (Table 2, column 4). The x coordinate of Be was assigned as 0.200 from consideration of interatomic distances. The residual factor for this set of coordinates is 0.44; the resulting electron-density map resolved all atoms in the structure, yielding the x coordinates of Table 4, column 2. A final electron-density projection (Fig. 1b) gave the x coordinates of Table 4, column 3.

Least-squares refinement of the atomic parameters, based on the data of the $hk0$ zone, gave the x coordinates of Table 4, columns 4

Table 4. *Atomic positional parameters, standard errors, and temperature coefficients for euclase*

Parameters		BISCOE and WARREN (1933)[1] (1)	Stage of refinement[2] (2)	(3)	(4)	(5) (final)	Standard errors in atomic parameters (in cycles)[3] (6)		Individual isotropic temperature coefficients B_j based on parameters of column (5) (7) hk0	(8) 0kl
Al	x	0.25	0.248	0.249	0.249	0.249	ε_x	0.0034		
	y	.44	.439	.443	.445	.4447	ε_y	.0040		
	z	.03	.946	.954	.956	.957	ε_z	.0052	0.10	0.19
Si	x	.15	.176	.177	.177	.177	ε_x	.0027		
	y	.10	.101	.100	.100	.1002	ε_y	.0030		
	z	.53	.546	.542	.540	.539	ε_z	.0039	.06	.00
O_1	x	.39	.378	.381	.380	.380	ε_x	.0067		
	y	.05	.036	.036	.032	.0321	ε_y	.0080		
	z	.78	.770	.761	.760	.761	ε_z	.0083	.18	.08
O_2	x	.39	.378	.383	.381	.380	ε_x	.0071		
	y	.35	.363	.374	.377	.3767	ε_y	.0080		
	z	.72	.643	.638	.650	.650	ε_z	.0090	.21	.16
O_3	x	.37	.347	.344	.346	.346	ε_x	.0062		
	y	.19	.196	.199	.200	.2000	ε_y	.0080		
	z	.46	.530	.525	.524	.520	ε_z	.0100	.20	.34
O_4	x	.17	.101	.101	.100	.100	ε_x	.0066		
	y	.03	.059	.051	.052	.0529	ε_y	.0080		
	z	.26	.236	.223	.222	.215	ε_z	.0100	.27	.21
O_5 (OH)	x	.18	.167	.158	.157	.158	ε_x	.0075		
	y	.33	.274	.330	.332	.3324	ε_y	.0100		
	z	.22	.957	.122	.116	.118	ε_z	.0116	.42	.39
Be	x	.48*	.193	.180	.177	.176	ε_x	.0164		
	y	.30	.250	.300	.301	.3000	ε_y	.0269		
	z	.50	.777	.478	.468	.470	ε_z	.0267	.46	.90
R	hk0		.300	.174	.148	.139				
	0kl		.552	.235	.177	.122				
B	hk0		.20	.09	.14	.15				
	0kl		.28	.18	.14	.14				

[1] Original parameters transferred to setting of present study.

[2] See text for the description of stage of refinement.

[3] For method of calculation see CLARK and CHRIST (1959).

R The residual factor; ΔF omitted in calculation if $F_{obs} = 0$.

B The average isotropic temperature coefficient (in Å^2).

ε_x The standard error in the positional parameter x of an atom.

* Possibly due to a misprint in BISCOE and WARREN's paper (1933).

and 5, after seven cycles of refinement with an overall temperature coefficient and seven additional cycles including individual isotropic temperature coefficients. Several small-angle reflections affected by

Table 5. *Comparison of observed and calculated structure factors for the hk*0 *and* 0*kl zones of euclase*

h	k	l	F_o	F_c
*2	0	0	–	-69
4	0	0	21	-29
6	0	0	10	9
8	0	0	9	9
10	0	0	–	-7
12	0	0	9	10
1	1	0	15	16
2	1	0	9	-8
3	1	0	15	-13
4	1	0	17	20
5	1	0	6	5
6	1	0	12	-12
7	1	0	6	-5
8	1	0	–	-3
9	1	0	–	-2
10	1	0	8	10
11	1	0	8	10
12	1	0	–	-4
13	1	0	3	-4
*0	2	0	–	44
1	2	0	4	5
2	2	0	14	-13
3	2	0	15	-15
4	2	0	12	11
5	2	0	19	21
6	2	0	23	-23
7	2	0	20	-20
8	2	0	13	12
9	2	0	13	13
10	2	0	–	4
11	2	0	–	-1
12	2	0	3	1
13	2	0	3	-4
1	3	0	10	7
2	3	0	21	-24
3	3	0	10	-9
4	3	0	21	23
5	3	0	8	5
6	3	0	11	-10
7	3	0	–	3
8	3	0	6	-6
9	3	0	9	-9
10	3	0	11	13
11	3	0	–	1
12	3	0	–	-3
13	3	0	6	8
0	4	0	20	-26
1	4	0	18	-15
2	4	0	14	12
3	4	0	32	-42
4	4	0	12	11
5	4	0	24	33
6	4	0	18	-18
7	4	0	15	-16
8	4	0	9	10
9	4	0	13	15
10	4	0	–	-1
11	4	0	9	-10
12	4	0	5	-2
13	4	0	–	-1
*1	5	0	–	-60
2	5	0	–	0
3	5	0	36	67
4	5	0	12	-11
5	5	0	15	-13
6	5	0	–	0
7	5	0	14	-12
8	5	0	9	9
9	5	0	10	10
10	5	0	–	1
11	5	0	–	-5
12	5	0	–	-3
13	5	0	–	2
0	6	0	17	-18
1	6	0	3	3
2	6	0	22	20
3	6	0	40	-60
4	6	0	15	-14
5	6	0	21	20
6	6	0	5	4
7	6	0	14	12
8	6	0	–	4
9	6	0	–	-1
10	6	0	–	-2
11	6	0	12	-13
12	6	0	10	-6
1	7	0	–	-1
2	7	0	11	10
3	7	0	–	-2
4	7	0	20	-21
5	7	0	–	0
6	7	0	8	6
7	7	0	5	4
8	7	0	8	8
9	7	0	–	0
10	7	0	6	-6
11	7	0	–	-5
12	7	0	–	3
0	8	0	31	-46
1	8	0	32	38
2	8	0	27	28
3	8	0	24	-25
4	8	0	17	-14
5	8	0	11	-10
6	8	0	13	11
7	8	0	20	19
8	8	0	9	-8
9	8	0	–	0
10	8	0	9	9
11	8	0	12	-13
12	8	0	–	-10
1	9	0	17	15
2	9	0	26	26
3	9	0	29	-30
4	9	0	13	-12
5	9	0	17	14
6	9	0	–	-2
7	9	0	6	7
8	9	0	–	-1
9	9	0	8	-7
10	9	0	–	1
11	9	0	–	1
12	9	0	–	7
0	10	0	–	0
1	10	0	20	-16
2	10	0	–	-2
3	10	0	11	7
4	10	0	24	-21
5	10	0	–	0
6	10	0	33	39
7	10	0	–	0
8	10	0	21	-23
9	10	0	–	-4
10	10	0	–	1
11	10	0	5	5
12	10	0	–	1
1	11	0	6	-4
2	11	0	23	21
3	11	0	10	-8
4	11	0	13	10
5	11	0	17	16
6	11	0	19	-19
7	11	0	–	-2
8	11	0	–	-1
9	11	0	6	-6
10	11	0	10	10
11	11	0	–	3
12	11	0	–	-4
0	12	0	29	-35
1	12	0	34	-45
2	12	0	7	6
3	12	0	26	22
4	12	0	8	6
5	12	0	–	2
6	12	0	16	15
7	12	0	–	-4
8	12	0	15	-16
9	12	0	6	-6
10	12	0	–	0
11	12	0	7	8
12	12	0	–	3
1	13	0	–	-2
2	13	0	23	-21
3	13	0	–	1
4	13	0	27	26
5	13	0	–	0
6	13	0	5	-4
7	13	0	–	3
8	13	0	14	-15
9	13	0	–	-1
10	13	0	9	9
11	13	0	–	-4
12	13	0	–	0
0	14	0	24	-30
1	14	0	27	-29
2	14	0	11	8
3	14	0	26	23
4	14	0	16	15
5	14	0	12	-10
6	14	0	12	-11
7	14	0	8	6
8	14	0	–	3
9	14	0	–	-5
10	14	0	–	-3
11	14	0	–	0
12	14	0	–	0
1	15	0	–	-2
2	15	0	5	3
3	15	0	20	17
4	15	0	–	2
5	15	0	24	-22
6	15	0	–	1
7	15	0	–	2
8	15	0	–	-3
9	15	0	15	15
10	15	0	–	-2
11	15	0	7	-8
12	15	0	–	1
0	16	0	–	0
1	16	0	8	-6
2	16	0	5	-2
3	16	0	13	10
4	16	0	13	11
5	16	0	7	-6
6	16	0	18	-19
7	16	0	7	7
8	16	0	13	13
9	16	0	13	-14
10	16	0	–	-4
11	16	0	7	8
12	16	0	–	1
1	17	0	17	13
2	17	0	27	27
3	17	0	9	-7
4	17	0	18	-16
5	17	0	16	-14
6	17	0	–	-1
7	17	0	5	5
8	17	0	6	6
9	17	0	9	9
10	17	0	7	-7
11	17	0	–	-3
0	18	0	21	22
1	18	0	26	26
2	18	0	19	-16
3	18	0	8	8
4	18	0	13	12
5	18	0	17	-17
6	18	0	11	-10
7	18	0	5	4
8	18	0	4	4
9	18	0	–	-1
10	18	0	–	-3
11	18	0	–	1
1	19	0	13	10
2	19	0	–	2
3	19	0	12	-11
4	19	0	–	-3
5	19	0	–	3
6	19	0	6	5
7	19	0	–	-2
8	19	0	–	-4
9	19	0	–	0
10	19	0	–	-3
11	19	0	7	7
0	20	0	30	30
1	20	0	16	15
2	20	0	22	-22
3	20	0	5	-3
4	20	0	8	7
5	20	0	–	0
6	20	0	6	5
7	20	0	7	-6
8	20	0	8	-7
9	20	0	8	7
10	20	0	5	-4
11	20	0	–	-2
1	21	0	11	9
2	21	0	17	-14
3	21	0	14	-13
4	21	0	–	3
5	21	0	6	5
6	21	0	4	2
7	21	0	–	0
8	21	0	6	5
9	21	0	5	-6
10	21	0	–	-1
11	21	0	6	7
0	22	0	–	-1
1	22	0	10	-9
2	22	0	–	-1
3	22	0	15	-13
4	22	0	8	6
5	22	0	22	21
6	22	0	8	-6
7	22	0	16	-15
8	22	0	–	-2
9	22	0	9	9
10	22	0	4	3
1	23	0	–	3
2	23	0	23	-24
3	23	0	–	-1
4	23	0	8	6
5	23	0	6	-5
6	23	0	8	7
7	23	0	–	2
8	23	0	–	1
9	23	0	–	3
10	23	0	–	0
0	24	0	–	-3
1	24	0	7	5
2	24	0	11	8
3	24	0	9	-8
4	24	0	12	-10
5	24	0	7	6
6	24	0	–	0
7	24	0	9	-9
8	24	0	7	6
9	24	0	11	13
10	24	0	–	0
1	25	0	12	-9
2	25	0	11	-10
3	25	0	19	17
4	25	0	–	0
5	25	0	11	-10
6	25	0	6	5
7	25	0	–	-4
8	25	0	–	1
9	25	0	9	11
10	25	0	–	1
0	26	0	17	-17
1	26	0	16	14
2	26	0	14	13
3	26	0	–	-3
4	26	0	8	-6
5	26	0	–	-4
6	26	0	–	1
7	26	0	–	-1
8	26	0	–	2
9	26	0	–	3
1	27	0	–	-3
2	27	0	11	9
3	27	0	–	-1
4	27	0	14	-11
5	27	0	9	7
6	27	0	–	2
7	27	0	–	3
8	27	0	7	7
9	27	0	8	-7
0	28	0	18	-16
1	28	0	8	7
2	28	0	9	7
3	28	0	–	3
4	28	0	–	-1
5	28	0	9	-8
6	28	0	7	7
7	28	0	6	6
8	28	0	8	-8
9	28	0	–	-2
1	29	0	8	-8
2	29	0	–	1
3	29	0	–	3
4	29	0	6	-6
5	29	0	15	13
6	29	0	5	6
7	29	0	5	-4
8	29	0	–	1
9	29	0	5	-9
0	30	0	15	13
1	30	0	7	-6
2	30	0	7	-6
3	30	0	–	5
4	30	0	12	-11
5	30	0	–	-4
6	30	0	18	19
7	30	0	6	6
8	30	0	7	-8
1	31	0	–	-2
2	31	0	5	-6
3	31	0	–	-2
4	31	0	8	6
5	31	0	8	9
6	31	0	–	0
7	31	0	–	-1
8	31	0	–	-2
0	32	0	–	3
1	32	0	12	-13
2	32	0	–	0
3	32	0	10	9
4	32	0	–	-2
5	32	0	–	0
6	32	0	5	-3
7	32	0	5	-1
1	33	0	–	2
2	33	0	–	-1
3	33	0	5	-3
4	33	0	9	10
5	33	0	–	0
6	33	0	5	-5
7	33	0	–	4
0	34	0	–	4
1	34	0	5	-6
2	34	0	–	0
3	34	0	9	10
4	34	0	–	1
5	34	0	–	-3
6	34	0	7	-9
1	35	0	7	-9
2	35	0	10	10
3	35	0	13	15
4	35	0	–	1
5	35	0	5	-5
6	35	0	–	-6
0	36	0	6	5
1	36	0	–	2
2	36	0	–	-3
3	36	0	–	0
4	36	0	3	4
5	36	0	–	-1
1	37	0	–	-1
2	37	0	6	8
3	37	0	–	2
4	37	0	4	-4
0	38	0	3	4
1	38	0	6	7
2	38	0	–	-3
3	38	0	6	-7
4	38	0	3	5
1	39	0	5	5
2	39	0	–	1
0	2	0	28	44
0	4	0	27	-27
0	6	0	18	-19
0	8	0	40	-46
0	10	0	–	0
0	12	0	30	-33
0	14	0	27	-30
0	16	0	–	0
0	18	0	21	22
0	20	0	29	29
0	22	0	–	0
0	24	0	–	-4
0	26	0	17	-18
0	28	0	14	-14
0	30	0	13	13
0	32	0	–	5
0	34	0	–	4
0	36	0	–	4
0	38	0	–	5
0	0	1	20	-28
0	1	1	10	6
0	2	1	32	42
0	3	1	27	26
0	4	1	30	34
0	5	1	10	7
0	6	1	20	18
0	7	1	20	-18
0	8	1	35	-39
0	9	1	18	15
0	10	1	54	-81
0	11	1	27	29
0	12	1	–	3
0	13	1	–	3
0	14	1	17	15
0	15	1	–	-1
0	16	1	21	21
0	17	1	–	2
0	18	1	25	21
0	19	1	7	-6
0	20	1	15	-13
0	21	1	7	-6
0	22	1	–	4
0	23	1	6	-6
0	24	1	–	5
0	25	1	10	-9
0	26	1	–	-3
0	27	1	–	-4
0	28	1	–	-5
0	29	1	–	-4
0	30	1	14	-15
0	31	1	–	-2
0	32	1	–	-3
0	33	1	8	7
0	34	1	9	9
0	35	1	8	9
0	36	1	11	15
0	37	1	–	1
0	38	1	5	4
0	39	1	–	0
0	0	2	39	44
0	1	2	37	-40
0	2	2	27	-23
0	3	2	21	-18
0	4	2	25	-24
0	5	2	33	36
0	6	2	27	-28
0	7	2	21	19
0	8	2	24	-22
0	9	2	4	4
0	10	2	33	34
0	11	2	13	-12
0	12	2	–	3
0	13	2	21	-20
0	14	2	–	-3
0	15	2	–	2
0	16	2	–	0
0	17	2	9	8
0	18	2	11	11
0	19	2	–	-4
0	20	2	29	32
0	21	2	–	1
0	22	2	–	0
0	23	2	–	4
0	24	2	14	-12
0	25	2	7	-6
0	26	2	14	-14
0	27	2	–	0
0	28	2	8	-6
0	29	2	–	6
0	30	2	10	9
0	31	2	–	-4
0	32	2	–	-5
0	33	2	–	-5
0	34	2	–	-7
0	35	2	–	-1
0	36	2	–	-4
0	37	2	–	3
0	38	2	–	0
0	39	2	–	8
0	0	3	29	-29
0	1	3	18	16
0	2	3	19	18
0	3	3	40	41
0	4	3	8	4
0	5	3	27	24
0	6	3	–	-2
0	7	3	21	-21
0	8	3	10	9
0	9	3	17	-17
0	10	3	32	-36
0	11	3	–	-2
0	12	3	14	-12
0	13	3	18	-15
0	14	3	19	14
0	15	3	20	-18
0	16	3	24	24
0	17	3	13	-12
0	18	3	8	7
0	19	3	–	-3
0	20	3	18	-18
0	21	3	21	21
0	22	3	–	2
0	23	3	24	25
0	24	3	–	6
0	25	3	9	10
0	26	3	–	5
0	27	3	–	1
0	28	3	–	-5
0	29	3	–	-5
0	30	3	15	-16
0	31	3	–	-6
0	32	3	–	6
0	33	3	–	-2
0	34	3	8	7
0	35	3	–	-4
0	36	3	–	1
0	37	3	–	-10
0	38	3	–	0
0	0	4	33	38
0	1	4	–	-3
0	2	4	23	22
0	3	4	11	6
0	4	4	14	14
0	5	4	23	22
0	6	4	23	-20
0	7	4	28	28
0	8	4	19	-20
0	9	4	14	15
0	10	4	10	8
0	11	4	24	-21
0	12	4	18	-16
0	13	4	33	-38
0	14	4	9	-7
0	15	4	21	-19
0	16	4	9	-8
0	17	4	10	9
0	18	4	–	-5
0	19	4	15	14
0	20	4	25	24
0	21	4	–	2
0	22	4	–	2
0	23	4	–	2
0	24	4	14	-13
0	25	4	11	10
0	26	4	–	-5
0	27	4	10	13
0	28	4	–	1
0	29	4	–	2
0	30	4	–	7
0	31	4	14	-13
0	32	4	–	2
0	33	4	12	-12
0	34	4	–	2
0	35	4	–	-2
0	36	4	–	4
0	37	4	–	4
0	0	5	9	-9
0	1	5	19	18
0	2	5	18	19
0	3	5	30	30
0	4	5	17	11
0	5	5	23	22
0	6	5	6	-6
0	7	5	8	6
0	8	5	7	-2
0	9	5	11	-10
0	10	5	23	-21
0	11	5	–	2
0	12	5	12	-8
0	13	5	12	14
0	14	5	–	4
0	15	5	–	-3
0	16	5	9	7
0	17	5	–	-22
0	18	5	–	
0	19	5	10	
0	20	5	–	
0	21	5	14	
0	22	5	–	
0	23	5	13	
0	24	5	–	
0	25	5	–	
0	26	5	–	
0	27	5	13	
0	28	5	–	
0	29	5	10	
0	30	5	10	
0	31	5	–	
0	32	5	–	
0	33	5	–	
0	34	5	–	
0	35	5	–	
0	36	5	–	
0	0	6	–	
0	1	6	–	
0	2	6	9	
0	3	6	–	
0	4	6	12	
0	5	6	7	
0	6	6	–	
0	7	6	27	
0	8	6	7	
0	9	6	16	
0	10	6	13	
0	11	6	18	
0	12	6	–	
0	13	6	17	
0	14	6	–	
0	15	6	9	
0	16	6	9	
0	17	6	9	
0	18	6	–	
0	19	6	15	
0	20	6	–	
0	21	6	10	
0	22	6	–	
0	23	6	14	
0	24	6	–	
0	25	6	–	
0	26	6	–	
0	27	6	13	
0	28	6	–	
0	29	6	10	
0	30	6	11	
0	31	6	–	
0	32	6	–	
0	33	6	–	
0	34	6	–	
0	35	6	–	
0	0	7	17	
0	1	7	19	
0	2	7	13	
0	3	7	22	
0	4	7	–	
0	5	7	–	
0	6	7	8	
0	7	7	9	
0	8	7	–	
0	9	7	11	
0	10	7	10	
0	11	7	–	
0	12	7	17	
0	13	7	–	
0	14	7	–	
0	15	7	10	
0	16	7	10	
0	17	7	11	
0	18	7	–	
0	19	7	–	
0	20	7	–	
0	21	7	14	
0	22	7	–	
0	23	7	11	
0	24	7	–	
0	25	7	9	
0	26	7	–	
0	27	7	6	
0	28	7	8	
0	29	7	9	
0	30	7	–	
0	31	7	–	
0	32	7	–	
0	33	7	–	
0	0	8	–	
0	1	8	9	
0	2	8	–	
0	3	8	–	
0	4	8	–	
0	5	8	13	
0	6	8	20	
0	7	8	–	
0	8	8	–	
0	9	8	–	
0	10	8	–	
0	11	8	–	
0	12	8	14	
0	13	8	–	
0	14	8	–	
0	15	8	–	
0	16	8	–	
0	17	8	–	
0	18	8	–	
0	19	8	8	
0	20	8	12	
0	21	8	–	
0	22	8	–	
0	23	8	8	
0	24	8	7	
0	25	8	8	
0	26	8	7	
0	27	8	6	
0	28	8	–	
0	29	8	5	
0	30	8	5	
0	31	8	–	

Table 5. *(Continued)*

h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c
0 0 9	12	12	0 15 9	8	- 7	0 1 10	9	- 8	0 16 10	6	2	0 6 11	-	- 5	0 0 12	13	- 13
0 1 9	11	12	0 16 9	7	- 7	0 2 10	6	- 10	0 17 10	6	5	0 7 11	8	- 6	0 1 12	-	- 2
0 2 9	-	3	0 17 9	8	- 6	0 3 10	-	- 3	0 18 10	-	- 2	0 8 11	9	- 12	0 2 12	4	- 5
0 3 9	17	18	0 18 9	-	2	0 4 10	-	7	0 19 10	-	- 2	0 9 11	7	- 9	0 3 12	-	1
0 4 9	8	- 8	0 19 9	-	- 6	0 5 10	-	4	0 20 10	-	- 2	0 10 11	16	16	0 4 12	5	6
0 5 9	11	9	0 20 9	-	2	0 6 10	-	8	0 21 10	-	- 7	0 11 11	-	2	0 5 12	-	- 3
0 6 9	-	0	0 21 9	-	5	0 7 10	-	4	0 22 10	7	- 1	0 12 11	-	6	0 6 12	6	8
0 7 9	-	- 2	0 22 9	-	1	0 8 10	-	4	0 23 10	-	- 5	0 13 11	-	1	0 7 12	-	- 5
0 8 9	-	5	0 23 9	-	4	0 9 10	10	8	0 24 10	-	4	0 14 11	-	- 4	0 8 12	9	6
0 9 9	-	1	0 24 9	7	1	0 10 10	-	- 3	0 0 11	-	- 2	0 15 11	-	4	0 9 12	-	2
0 10 9	-	3	0 25 9	-	1	0 11 10	-	1	0 1 11	-	- 1	0 16 11	-	- 5	0 10 12	-	- 1
0 11 9	9	10	0 26 9	-	2	0 12 10	-	6	0 2 11	7	- 6	0 17 11	-	0	0 11 12	-	- 2
0 12 9	-	2	0 27 9	-	4	0 13 10	-	4	0 3 11	-	- 3	0 18 11	4	- 2	0 12 12	4	- 3
0 13 9	-	- 1	0 28 9	-	2	0 14 10	-	8	0 4 11	8	- 12	0 19 11	-	- 6	0 13 12	-	- 5
0 14 9	10	- 10	0 0 10	14	- 16	0 15 10	-	1	0 5 11	-	0	0 20 11	-	1			

Omitted from least-squares refinement

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extinction were not included in the least-squares refinement. The *y* coordinates obtained from the refinement of the two zones of data are virtually identical. The standard errors in atomic parameters are given in Table 4, column 6. Observed and calculated structure factors for the $hk0$ and $0kl$ zones of euclase are listed in Table 5. The final residual factors are $R_{hk0} = 0.14$ and $R_{0kl} = 0.12$.

Description of the structures

A. Väyrynenite

The crystal structure of väyrynenite consists of zigzag chains with composition $[Be_2(OH)_2(PO_4)_2]_n^{-4n}$ (Fig. 2a) cross-linked by Mn atoms between the chains and by hydrogen bonds. There are two crystallographically equivalent chains in the unit cell, oriented parallel to [100], and related to each other by a center of symmetry so that the *b* cell dimension represents two chain-widths. The Mn atoms lie between the chains and are octahedrally coordinated by two oxygen atoms and one hydroxyl oxygen from one chain (O_1, O_2, O_5,) and by one oxygen atom from each of three adjacent chains (O_1', O_4', O_4), as shown in Figs. 1a and 1c.

Within the $[Be_2(OH)_2(PO_4)_2]_n^{-4n}$ chain (Fig. 1a) each Be atom is tetrahedrally coordinated by two oxygen atoms (O_2, O_3') and by two hydroxyl oxygens (O_5, O_5'); each P atom is tetrahedrally coordinated by four oxygen atoms (O_1, O_2, O_3, O_4). The characteristic features of the chain are as follows: (1) PO_4 tetrahedra do not share corners with other PO_4 tetrahedra, but share two oxygen atoms with two adjacent $BeO_2(OH)_2$ tetrahedra; (2) no oxygen atom is shared by more than two tetrahedra; (3) all four corners of the $BeO_2(OH)_2$ tetrahedron are shared, two with adjacent $BeO_2(OH)_2$ tetrahedra and two with PO_4 tetrahedra, thereby forming a puckered six-membered ring consisting of $Be-O_2-P-O_3-Be-O_5'$ (Fig. 1a); (4) the hydroxyl oxygen, O_5, is shared between two $BeO_2(OH)_2$ tetrahedra.

The identification of O_5 as the hydroxyl oxygen was originally made from the fact that O_5 is the only oxygen atom in the structure which is not part of the tightly bonded PO_4 complex. The distance of 2.76 Å between O_5 and O_3' (Fig. 1c) shows the presence of a hydrogen bond (PIMENTEL and McCLELLAN, 1960, p. 260). Calculation of bond strengths based on a simple model (Table 6), assuming: (1) all Mn-O bonds $= \frac{1}{3}$, (2) all P-O bonds $= 1\frac{1}{4}$, (3) all Be-O bonds $= \frac{1}{2}$, shows
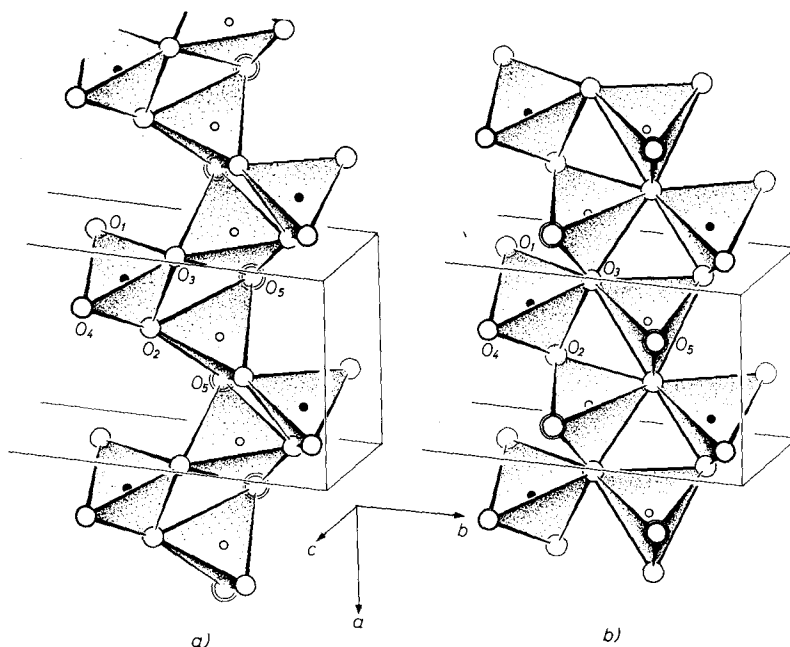
Fig. 2. A comparison of the $[Be_2(OH)_2(PO_4)_2]_n^{-4n}$ chain of väyrynenite (a) with the $[Be_2(OH)_2(SiO_4)_2]_n^{-6n}$ chain of euclase (b): large single circles, oxygen; large double circles, hydroxyl oxygen; small open circles, beryllium; small solid circles, silicon or phosphorus.

that local charge balance is maintained if the hydrogen bond is assigned a strength of $\frac{1}{3}$. This value is consistent with the average O-H distance of 1.0 Å given by PIMENTEL and McCLELLAN (1960) for hydrogen bonds with O-O distances in the neighborhood of 2.76 Å.

The perfect {010} cleavage of väyrynenite (MROSE and VON KNORRING, 1959) is between the chains and requires breaking only four Mn-O bonds for each unit cell; the good but difficult {100} cleavage is normal to the chains and requires breaking two Be-OH bonds, two Be-O or

Table 6. *Summary of approximate bond strengths in väyrynenite and euclase*

The following bond strengths are assumed: Mn—O = 1/3, Al—O = 1/2,
P—O = 5/4, Si—O = 1, Be—O = 1/2; väyrynenite, H—O₃ = 1/3, H—O₅* = 2/3.

Compound	Anion	Coordinated cations	Sum of bond strengths
Väyrynenite	O_1, O_4	2 Mn, 1 P	1.92
Euclase	O_1, O_4	2 Al, 1 Si	2.00
Väyrynenite	O_2	1 Mn, 1P, 1 Be	2.08
Euclase	O_2	1 Al, 1 Si, 1 Be	2.00
Väyrynenite	O_3	1 P, 1 Be, (1 H)	1.75, (2.08)
Euclase	O_3	1 Si, 2 Be	2.00
Väyrynenite	O_5*	1 Mn, 2 Be, (1 H)	1.33, (2.00)
Euclase	O_5*	1 Al, 1 Be, (1 H)	1, (2.00)

* Hydroxyl oxygen.

P-O bonds, and four Mn-O bonds; the fair {001} cleavage is between
the chains but requires breaking eight Mn-O bonds and four hydrogen
bonds. The observed order of the cleavages is in agreement with the
bond strengths calculated on the basis of the charge balance discussed
above.

Interatomic distances and bond angles found in väyrynenite are
listed in Tables 7 and 8, together with standard errors calculated by
the method described in CLARK, CHRIST, and APPLEMAN (1962).
The average P-O distance in the PO_4 tetrahedron is 1.53 Å; for com-
parison, the average P-O distance found in the well refined $LiMnPO_4$
structure (GELLER and DURAND, 1960) is 1.54 Å for discrete PO_4
tetrahedra. Although the shortest tetrahedral P-O distances in väyryne-
nite, as would be expected, are those involving oxygens not shared
with $BeO_2(OH)_2$ tetrahedra, the differences in bond lengths within
the PO_4 tetrahedron may not be significant in view of the standard
errors given in Table 7. The distortion of the PO_4 tetrahedron shown
by the O-P-O angles listed in Table 8 is apparently real, and similar
distortion has been reported in several recent studies of phosphate
structures, summarized by GELLER and DURAND (1960).

The $BeO_2(OH)_2$ tetrahedron is not as regular as the PO_4 tetrahe-
dron; the most noticeable distortion in the former is the length of the
edge between the hydroxyl oxygens. The average tetrahedral Be-O
distance of 1.65 Å found here is the same as the average Be-O distance

Table 7. *Interatomic distances and standard errors in väyrynenite and euclase*
(See Fig. 1)

Väyrynenite		Euclase	

Distances in tetrahedron around Be

Väyrynenite		Euclase	
Be—O_2	1.63 Å	Be—O_2	1.60 Å
Be—O_5'*	1.69	Be—O_3	1.63
Be—O_3'	1.65	Be—O_3'	1.64
Be—O_5*	1.63	Be—O_5*	1.68
Average	1.65$_0$ Å	Average	1.63$_8$ Å
Be—O bonds	± 0.03$_1$ Å	Be—O bonds	± 0.04$_4$ Å

Distances in tetrahedra around P and Si

Väyrynenite		Euclase	
P—O_1	1.53 Å	Si—O_1	1.61 Å
P—O_2	1.53	Si—O_2	1.62
P—O_3	1.55	Si—O_3	1.65
P—O_4	1.51	Si—O_4	1.62
Average	1.53$_0$ Å	Average	1.62$_5$ Å
P—O bonds	±0.01$_5$ Å	Si—O bonds	± 0.01$_5$ Å

Distances in octahedra around Mn and Al

Väyrynenite		Euclase	
Mn—O_1	2.08 Å	Al—O_1	1.86 Å
Mn—O_1'	2.24	Al—O_1'	1.98
Mn—O_4	2.14	Al—O_4	1.87
Mn—O_4'	2.18	Al—O_4'	1.93
Mn—O_2	2.23	Al—O_2	1.91
Mn—O_5*	2.37	Al—O_5*	1.85(± 0.01$_9$ Å)
Average	2.20$_7$ Å	Average	1.90$_0$ Å
Mn—O bonds	± 0.01$_5$ Å	Al—O bonds	± 0.01$_6$ Å
		(excluding Al—O_5)	

Oxygen-oxygen distances for oxygens bonded to the same Be

Väyrynenite		Euclase	
O_2–O_3'	2.64 Å	O_2–O_3'	2.59 Å
O_2–O_5*	2.58	O_2–O_5*	2.57
O_2–O_5'*	2.72	O_2–O_3	2.74
O_3'–O_5*	2.73	O_3'–O_5*	2.69
O_3'–O_5'*	2.65	O_3–O_5*	2.62
O_5*–O_5'*	2.81	O_3'–O_3	2.78
Average	2.68$_8$ Å	Average	2.66$_5$ Å

Table 7. *(Continued)*

Väyrynenite		Euclase	

Oxygen-oxygen distances for oxygens bonded to the same P or Si

O_1–O_2	2.52 Å	O_1–O_2	2.68 Å
O_1–O_3	2.50	O_1–O_3	2.64
O_1–O_4	2.52	O_1–O_4	2.65
O_3–O_3	2.48	O_2–O_3	2.64
O_3–O_4	2.48	O_2–O_4	2.63
O_3–O_4	2.50	O_3–O_4	2.68
Average	2.50_0 Å	Average	2.65_3 Å

Oxygen-oxygen distances for oxygens bonded to the same Mn or Al

O_1–O_1'	2.72 Å	O_1–O_1'	2.47 Å
O_1–O_2	3.63	O_1–O_2	2.84
O_1–O_4'	3.20	O_1–O_4'	2.74
O_1–O_5*	3.28	O_1'–O_5*	2.73
O_1'–O_4	2.94	O_1'–O_4	2.61
O_1'–O_4'	2.99	O_1'–O_4'	2.69
O_1'–O_5*	4.09	O_1'–O_5*	2.92
O_2–O_4	2.93	O_2–O_4	2.82
O_2–O_4'	2.89	O_2–O_4'	2.59
O_2–O_5*	2.58	O_2–O_5*	2.65
O_4–O_4'	2.92	O_4–O_4'	2.54
O_4–O_5*	3.26	O_4–O_5*	2.64
Average	3.11_9 Å	Average	2.68_7 Å

Distances between oxygen atoms not bonded to the same cation (only distances
< 3.00 Å listed)

O_5*–O_3'	2.76 Å	O_3–O_5*	2.93 Å

hydrogen bond

(between chains)

0—O distances ± 0.02_1 Å

(between chains)

O—O distances (excluding O—O_5*)
± 0.02_0 Å; O—O_5* distances
± 0.02_2 Å

* Hydroxyl oxygen.

found by JEFFREY, PARRY, and MOZZI (1956) in hexagonal beryllium
oxide, which has a wurtzite-type structure. The octahedron around
the Mn atom in väyrynenite is highly distorted; individual O-Mn-O
angles deviate as much as 35° from the average of 90.8°.

Table 8. *Bond angles and standard errors in väyrynenite and euclase*
(See Fig. 1)

Väyrynenite		Euclase	

Bond angles in tetrahedron around Be

Väyrynenite		Euclase	
O_2—Be—O_3'	107.6°	O_2—Be—O_3'	106.6°
O_2—Be—O_5*	104.6	O_2—Be—O_5*	103.7
O_2—Be—O_5'*	110.8	O_2—Be—O_3	116.1
O_3'—Be—O_5*	112.9	O_3'—Be—O_5*	108.4
O_3'—Be—O_5'*	105.1	O_3—Be—O_5*	104.5
O_5*—Be—O_5'*	115.8	O_3—Be—O_3'	116.5
Average	109.5°	Average	109.3°
O—Be—O angles	± 1.0°	O—Be—O angles	± 1.5°

Bond angles in tetrahedra around P and Si

Väyrynenite		Euclase	
O_1—P—O_2	110.9°	O_1—Si—O_2	112.4°
O_1—P—O_3	108.5	O_1—Si—O_3	108.3
O_1—P—O_4	111.8	O_1—Si—O_4	110.4
O_2—P—O_3	107.3	O_2—Si—O_3	107.6
O_2—P—O_4	109.0	O_2—Si—O_4	108.0
O_3—P—O_4	109.2	O_3—Si—O_4	110.1
Average	109.5°	Average	109.5°
O—P—O angles	± 0.7°	O—Si—O angles	± 0.7°

* Hydroxyl oxygen

B. Euclase

The crystal structure of euclase consists of zigzag chains with composition $[Be_2(OH)_2(SiO_4)_2]_n^{-6n}$ (Fig. 2b) cross-linked by Al atoms between the chains. The chains are oriented parallel to [100], and are disposed in the unit cell in the same way as those of väyrynenite. The Al atoms between the chains are octahedrally coordinated by two oxygen atoms from one chain (O_1, O_2), by one oxygen atom (O_4) and one hydroxyl oxygen (O_5) from one adjacent chain, and by one oxygen atom from each of two different neighboring chains (O_1', O_4'), as shown in Figs. 1b and 1d.

Within the $[Be_2(OH)_2(SiO_4)_2]_n^{-6n}$ chains (Fig. 1b) each Be atom is tetrahedrally coordinated by three oxygen atoms (O_2, O_3, O_3') and by one hydroxyl oxygen (O_5); each Si is tetrahedrally coordinated by four oxygen atoms (O_1, O_2, O_3, O_4). The characteristic features of the

chain are as follows: (1) SiO_4 tetrahedra do not share corners with
other SiO_4 tetrahedra, but share two oxygen atoms with three adjacent
$BeO_3(OH)$ tetrahedra; this follows from the fact that (2) one oxygen
atom, O_3, is shared by one SiO_4 and two $BeO_3(OH)$ tetrahedra; (3)
three corners of the $BeO_3(OH)$ tetrahedron are shared, two with
adjacent $BeO_3(OH)$ tetrahedra and one with the SiO_4 tetrahedron,
thus forming a puckered six-membered ring consisting of Be-O_2-Si-O_3-
Be-O_3' (Fig. 1b); and (4) the fourth corner of the $BeO_3(OH)$ tetrahedron,
which is the hydroxyl oxygen O_5, is not shared with any other tetrahe-
dron.

The hydroxyl oxygen was originally identified with O_5 from the
fact that O_5 is the only oxygen atom in the structure which is not part
of the tightly bonded SiO_4 complex. The shortest approach of this
atom to any oxygen atom not included in the same coordination
polyhedron is the 2.93 Å distance between O_5 and O_3 (Fig. 1d). In the
absence of other evidence, this distance is too long to be indicative of
hydrogen bonding (PIMENTEL and MCCLELLAN, 1960, p. 260). Calcula-
tions of bond strengths based on a simple model (Table 6), assuming:
(1) all Al-O bonds $= \frac{1}{2}$, (2) all Si-O bonds $= 1$, and (3) all Be-O bonds
$= \frac{1}{2}$, show that local charge balance is maintained if the proton is
associated entirely with O_5.

The sharing of one oxygen atom between three separate tetrahedral
groups, in the manner that O_3 in the euclase structure is shared be-
tween one SiO_4 and two $BeO_3(OH)$ tetrahedra, is not a common struc-
tural arrangement. However, precisely the same linkage occurs in the
structure proposed by BRAGG and ZACHARIASEN (1930) for phenacite,
Be_2SiO_4. In that structure every oxygen atom is likewise bonded to
one SiO_4 tetrahedron and two BeO_4 tetrahedra.

The perfect {010} cleavage of euclase (MROSE and VON KNORRING,
1959), as in the case of väyrynenite, is between the chains in the struc-
ture and requires breaking only four Al-O bonds for each unit cell.
The crystals of euclase used in the present study also have a good {100}
cleavage, moderately easy to produce, and a fair but very difficult
{001} cleavage. The {100} cleavage across the chains requires breaking
four Be-O bonds or two Be-O and two Si-O bonds, and four Al-O
bonds; the {001} cleavage between the chains requires breaking 12
Al-O bonds. The observed order of the cleavages is in accord with bond
strengths calculated on the basis of the charge balance discussed above.

The structure found for euclase in the present study is essentially
that proposed by BISCOE and WARREN (1933) and illustrated in Fig. 1b

of their paper. That figure, labeled "projected upon (a, b) plane", should actually be labeled "projected upon (b, c) plane". It corresponds to a projection on the (001) plane in the setting of the present study. An erroneous x coordinate (0.48) is listed for Be (Table 4, column 1) and was used in Fig. 2 of BISCOE and WARREN (1933). With this exception, the atomic coordinates derived by those authors (Table 4, column 1) are in reasonable agreement with those obtained in the present work (Table 4, column 5).

Interatomic distances and bond angles obtained in the present study of euclase are listed in Tables 7 and 8, arranged for comparison with corresponding distances and angles found in väyrynenite. Standard errors were calculated by the method described in CLARK, CHRIST, and APPLEMAN (1962). The average Si-O distance in the SiO_4 tetrahedron is 1.62_5 Å, in good agreement with the average distances of 1.62_6 Å and 1.63_7 Å reported by SMITH, KARLE, HAUPTMAN, and KARLE (1960) for the two independent SiO_4 tetrahedra in spurrite, $Ca_5(SiO_4)_2CO_3$. The distortion induced in the SiO_4 tetrahedron of euclase by the long $Si-O_3$ distance is probably real; it is not unexpected, since O_3 is the only oxygen in the SiO_4 tetrahedron shared with two $BeO_3(OH)$ tetrahedra. The range of the remaining Si-O distances is within the standard error of the determination. The $BeO_3(OH)$ tetrahedron is also distorted, principally owing to the long $Be-O_5$ distance. The average Be-O distance in the tetrahedron, 1.64 Å, is virtually the same as that found in väyrynenite. The octahedron around the Al atom in euclase is fairly regular, with a maximum deviation of 9.5° from the average O-Al-O angle of 90.1°. The average Al-O distance of 1.90_2 Å is comparable to the average distance of 1.915 Å found by BUSING and LEVY (1958) in diaspore, AlO(OH).

Comparison of the structures

A comparison of the crystal structures of väyrynenite and euclase (Fig. 1, Tables 2 and 4), shows that the arrangement of PO_4 tetrahedra around Mn in väyrynenite is almost identical with the arrangement of SiO_4 tetrahedra around Al in euclase. The differences between the two structures are chiefly a consequence of the change in electrostatic charge distribution induced by the replacement of Al^{+3} by Mn^{+2} in an octahedrally-coordinated site, and of Si^{+4} by P^{+5} in a tetrahedrally-coordinated site. In order to maintain local charge balance, the positions of Be and OH in väyrynenite must necessarily be quite different from those in euclase. This requirement is apparent from an analysis

of Table 6, where the approximate bond strengths in the two structures are given, calculated on the basis of a simple model.

The sums of the strengths of the bonds terminating on oxygen atoms O_1, O_2, and O_4 are almost the same for a structure containing Mn and P as for one containing Al and Si, owing to the fact that these oxygen atoms coordinate both the octahedral and the tetrahedral sites. However, oxygen atom O_3 coordinates the tetrahedral but not the octahedral site, whereas hydroxyl oxygen O_5 coordinates the octahedral but not the tetrahedral site. In order to maintain local charge balance O_3 must form one Be-O bond in väyrynenite and two Be-O bonds in euclase; O_5 must form two Be-O bonds in väyrynenite and one Be-O bond in euclase. This can be accomplished only if both the Be and the O_5 positions are different in the two structures.

As a result of these differences in Be and O_5 positions, the chains in euclase do not have exactly the same configuration as those in väyrynenite. In a single euclase chain (Fig. 2b) the apices of the PO_4 tetrahedra, O_4, and of the $BeO_3(OH)$ tetrahedra, O_5, all point in approximately the same direction; but in väyrynenite (Fig. 2a) the O_5-O_5 edges of the $BeO_2(OH)_2$ tetrahedra project from the chain in the opposite direction from the apices, O_4, of the PO_4 tetrahedra. The väyrynenite configuration permits the formation of inter-chain hydrogen bonds between O_3 and the hydroxyl oxygen O_5 (Fig. 1a), thus restoring local charge balance around these two atoms (Table 8).

The cleavages in väyrynenite and euclase, as described in the previous sections, are entirely comparable. The crystal habits of the two minerals, however, differ in one important respect. Euclase crystals are elongated parallel to [100], the direction of the chain axes, whereas väyrynenite crystals are elongated parallel to [001] (MROSE and VON KNORRING, 1959), the direction of strongest interchain bonding. Although euclase also has strong interchain bonding parallel to [001], it lacks the hydrogen bonding approximately parallel to [001], described above in väyrynenite. The difference in hydrogen bonding in the two structures apparently gives rise to the difference in elongation direction of the crystals.

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