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CRYSTAL STRUCTURE OF REEDMERGNERITE, A BORON ALBITE, AND ITS RELATION TO FELDSPAR CRYSTAL CHEMISTRY[1]

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ABSTRACT

Reedmergnerite, $NaBSi_3O_8$, which is isostructural with low albite, $NaAlSi_3O_8$, is triclinic $C\bar{1}$, $a=7.833\pm0.001$, $b=12.360\pm0.002$, $c=6.803\pm0.001$ Å, $\alpha=93°18.5'\pm0.7'$; $\beta=116°, 21.1'\pm0.5'$, $\gamma=92°03.3'\pm0.8'$, cell volume 587.77 ± 0.05 Å^3, cell contents $4(NaBSi_3O_8)$, density (calc.) 2.779 g/cm^3, (obs.) 2.776 ± 0.010. Least-squares refinement has been carried out for three-dimensional data, collected by film methods, with intensities estimated partly by photometer and partly visually. The R-factor is 0.109 for 2997 structure factors observed greater than zero. The structure is wholly ordered, with the boron in site $T_1(0)$. The average Si-O distances in reedmergnerite are, $T_1(m)$ 1.610, $T_2(0)$ 1.614, $T_2(m)$ 1.622 Å, and the individual distances correlate closely with the corresponding ones in low albite (Ribbe *et al.*, 1952). Smith's curve, modified by Smith and Bailey (1963), for determination of Al-content from average T-O distance has an error approaching $\pm 8\%$, rather than the $\pm 5\%$ proposed by Smith and Bailey. The results for reedmergnerite, compared with those for low albite, maximum microcline (Brown and Bailey, 1964), and anorthite (Megaw *et al.*, 1962), suggest that Al-O tetrahedra deviate from regularity more than either B-O or Si-O tetrahedra. The sodium cation in reedmergnerite has an isotropic temperature factor of 1.22 ± 0.03 Å^2, and, in contrast to the sodium cation in low albite, exhibits no apparent anisotropy.

INTRODUCTION

The mineral reedmergnerite was found to be isostructural with low albite (Milton *et al.* 1954) at about the same time that the first information became available on the two-dimensional refinement of the low albite structure by Ferguson *et al.* (1954). A unique opportunity appeared to have been provided by Nature to obtain additional information about the feldspar structure type through study of reedmergnerite, so we began collection of single-crystal, three-dimensional, *x*-ray diffraction data for this new mineral.

The final report on the two-dimensional refinement of low albite by Ferguson *et al.* appeared in 1958, and included two principal points of interest: (1) the marked anisotropy found for the sodium cation; (2) the high degree of ordering indicated for Si and Al atoms in the tetrahedral sites. With respect to the latter, Ferguson *et al.* (1958) used their evaluation of electrostatic charge balance in the structure, together with the relationship proposed by Smith (1954) between mean Si-O distance and Si/Al site occupancy, as evidence for the following tetrahedral site Al-

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[1] Studies of silicate minerals (I). Publication authorized by the Director, U. S. Geological Survey.

occupancy factors: $T_1(0)$, 0.72; $T_1(m)$, 0; $T_2(0)$, 0.20; $T_2(m)$, 0.09. Preliminary results of a partial refinement of the reedmergnerite data (Clark and Appleman, 1960) showed that these same charge balance considerations could not be applied in a meaningful way to the reedmergnerite structure, and that Smith's relationship required revision. We therefore suggested that such considerations should be regarded cautiously in drawing conclusions about Si/Al ordering in the feldspar structure.

Refinement of three-dimensional data for the low albite structure has now been completed, but as of this writing only a preliminary note by Ribbe *et al.* (1962) has appeared. The anisotropy of the sodium cation is confirmed, and an ordered Si/Al distribution in the tetrahedral sites is indicated. Further details are as yet unavailable. Meanwhile, our refinement of the reedmergnerite data has been completed, and the present paper records our results and conclusions. We have used the coordinates for low albite given by Ribbe *et al.* (1962) to calculate distances and angles in order to compare some details of the two structures.

EXPERIMENTAL WORK

Synthesis, crystallography and X-ray diffraction powder data. The synthesis of reedmergnerite and temperatures for its incongruent melting to quartz and glass have been described by Eugster and McIver (1959). The synthetic crystals, made available to us by Prof. H. P. Eugster of The Johns Hopkins University, are tiny and invariably twinned, so they were not used in the structure study. A detailed comparison of *x*-ray powder diffraction patterns of synthetic reedmergnerite with those of natural reedmergnerite reveals no significant differences in line positions or intensities. The synthetic material appears to be identical with the natural crystals. Some experiments on heating natural reedmergnerite crystals were carried out by B. J. Skinner of the U. S. Geological Survey, who found that incongruent melting, dry, occurs at 831°±4° C. with the products quartz, glass and tridymite. No change was observed in the natural crystals after dry heating up to 816° C. for as long as 40 hours (B. J. Skinner, written comm., 1961). Apparently there is no readily obtainable high-temperature form of reedmergnerite, comparable to high-temperature albite.

For the structural study, natural prismatic crystals of dimensions approximately $0.5\times0.4\times0.3$ mm were used. These crystals originated in brown, dolomitic shales of the Green River Formation in Duchesne County, Utah, U.S.A., and were supplied by Charles Milton of the U. S. Geological Survey. Optical, chemical, and morphological data for reedmergnerite are given by Milton *et al.* (1960). Revised cell constants for

Table 1. Crystallographic Data for the Triclinic, Isostructural Minerals Reedmergnerite, $NaBSi_3O_8$, and Low Albite, $NaAlSi_3O_8$

	Reedmergnerite Duchesne County, Utah Present study	Low albite[1] Ramona, Calif. Ferguson *et al.* (1958)
Direct-cell elements		
a	7.833±0.001 Å	8.138 Å
b	12.360±0.002	12.789
c	6.803±0.001	7.156
α	93°18.5′±0.7′	94° 20′
β	116°21.1′±0.5′	116° 34′
γ	92°03.3′±0.8′	87° 39′
$a:b:c$	0.6337:1:0.5504	[0.6363:1:0.5595]
Volume	587.77±0.05 Å^3	664.2 Å^3
Z	4($NaBSi_3O_8$)	4($NaAlSi_3O_8$)
Space group	$C\bar{1}$	$C\bar{1}$
Density (calc.)	2.779 g/cm^3	2.623 g/cm^3
(obs.)	2.776±0.010	2.621
Reciprocal-cell elements		
a^*	0.14281±0.00002 Å^{-1}	[0.1374 Å^{-1}]
b^*	0.08124±0.00001	[0.07842]
c^*	0.16460±0.00001	[0.1566]
α^*	85°17.0′±0.6′	86°20′±2′
β^*	63°27.0±0.5′	63°32′±2′
γ^*	86°3.6′±0.7′	90°28′±2′
Direct matrix (Å)		
for conversion of triclinic cell elements to Cartesian coordinates (Evans, 1948)	$\begin{vmatrix} 7.019 & -0.848 & 0 \\ 0 & 12.310 & 0 \\ -3.477 & -0.713 & 6.803 \end{vmatrix}$	$\begin{vmatrix} 7.279 & 0.103 & 0 \\ 0 & 12.752 & 0 \\ -3.640 & -0.966 & 7.156 \end{vmatrix}$

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[1] Values enclosed in square brackets and the direct matrix have been calculated by present authors from the data of Ferguson *et al.* (1958).

reedmergnerite (Table 1) were obtained during the present study from a least-squares program (Evans, Appleman and Handwerker, 1963) for a digital computer. The program refined measurements made by T. L. Wright of the U. S. Geological Survey, from an *x*-ray diffractometer powder pattern for unambiguously indexed d-spacings. The revised direct-cell and reciprocal-cell elements for reedmergnerite are compared in Table 1 with those given for low albite by Ferguson, Traill and Taylor (1958). The $C\bar{1}$ space group commonly used for albite has been adopted for reedmergnerite throughout the present study. The x-ray diffraction powder data for reedmergnerite, indexed on the $C\bar{1}$ cell, are presented in Table 2.

The observed density of reedmergnerite crystals was reported by Milton *et al.* (1960) to be 2.69 g/cm³, whereas the calculated x-ray density (Table 1) is 2.779 g/cm³. In the present study, when the density of a sample of cloudy to opaque crystals was determined on a Berman balance, the 2.69 g/cm³ value was also found. However, when a sample of about 8 mg of selected transparent crystals was used for the determination, an observed density of 2.77_6 g/cm³ was found, in good agreement with the

TABLE 2. X-RAY DIFFRACTION POWDER DATA FOR REEDMERGNERITE, $NaBSi_3O_8$

Triclinic, $C\bar{1}$: $a=7.833\pm0.001$, $b=12.360\pm0.002$, $c=6.803\pm0.001$ Å,
$\alpha=93°18.5'\pm0.7'$, $\beta=116°21.1'\pm0.5'$, $\gamma=92°3.3'\pm0.8'$

Calculated[1]		Measured[2]	
hkl	d_{hkl} (Å)	d_{hkl} (Å)	Peak Height[3]
$\bar{1}10$	6.274	6.270	10
020	6.155	6.143	15
001	6.075	6.076	50
110	5.914		
$\bar{1}\bar{1}1$	5.550	5.551	20
$\bar{1}11$	5.449		
$0\bar{2}1$	4.513		
021	4.156		
$\bar{2}01$	3.874	3.876	65
$1\bar{1}1$	3.745	3.745	30
$\bar{1}30$	3.651	3.654	35
111	3.560	3.561	90
200	3.501		
$\bar{1}\bar{3}1$	3.449	3.448	15
130	3.439		
$\bar{1}31$	3.377		
$\bar{1}\bar{1}2$	3.323	3.322	15
$\bar{2}21$	3.314		
$\bar{2}\bar{2}1$	3.244		
$\bar{1}12$	3.225	3.225	85
$\bar{2}20$	3.137	3.140	25
040	3.077	3.076	90
$\bar{2}02$	3.073		
002	3.038	3.037	100
220	2.957	2.957	45
$1\bar{3}1$	2.930	2.931	15
$0\bar{4}1$	2.841	2.841	55
$0\bar{2}2$	2.817	2.818	35
$\bar{2}\bar{2}2$	2.775	2.776	5
$\bar{2}22$	2.725		
$1\bar{3}2$	2.695		

[1] All calculated d_{hkl} are listed for $d\geq2.300$ Å; for $d<2.300$ Å only those indexing observed lines are given.

[2] Diffractometer pattern made by T. L. Wright with Ni-filtered Cu radiation, $CuK\alpha_1$, $\lambda=1.5405$ Å. Internal standard, CaF_2 ($a=5.4622$ Å).

[3] Estimated above average background.

TABLE 2—(*continued*)

Calculated[1]		Measured[2]	
hkl	d_{hkl} (Å)	d_{hkl} (Å)	Peak Height[3]
131	2.680	2.680	45
041	2.659		
022	2.639		
201	2.576		
$\bar{3}11$	2.568		
$\bar{1}32$	2.544	2.543	5
$\bar{3}11$	2.525		
$2\bar{2}1$	2.452	2.452	10
$\bar{2}41$	2.438	2.438	10
$1\bar{1}2$	2.415	2.415	20
$\bar{3}12$	2.411		
$\bar{3}\bar{1}2$	2.405		
$\bar{2}40$	2.394		
$\bar{2}\bar{4}\bar{1}$	2.382	2.382	15
$\bar{1}50$	2.374		
112	2.335		
$\bar{3}10$	2.323		
221	2.307	2.307	5
$\bar{1}\bar{5}1$	2.304		
240	2.236	2.238	15
$\bar{1}\bar{1}3$	2.221	2.221	20
$\bar{1}13$	2.168	2.169	10
$2\bar{4}1$	2.064	2.064	15
060	2.052	2.053	10
$\bar{1}\bar{5}2$	2.051		
003	2.025	2.025	15
$\bar{3}13$	2.013	2.013	10
132	2.007	2.008	5
		plus others, all 30 or less	

calculated value. The presence of air-containing inclusions and other imperfections in the cloudy and opaque crystals probably explains observation of the lower value when a bulk sample is used.

Intensity data. Single-crystal *x*-ray diffraction data were collected by integrated multiple-film techniques with the Nonius equi-inclination Weissenberg goniometer using chiefly Zr-filtered Mo radiation. A few low-angle reflections were recorded using Ni-filtered Cu radiation. The *hnl* levels from $n=0$ through $n=8$ were photographed, two goniometer settings being required for each upper level in order to cover the full 360° range. The *hk*0 and 0*kl* nets were also recorded. For the Mo photographs, three films interleaved with 0.0005 in. Ni foil were used for each exposure, and for each goniometer setting, two sets of films were recorded, one set for 2520 traverses of the camera, and one set for 140 traverses of the camera. These numbers of traverses correspond to exposure times of approximately 72 hours and 4 hours, respectively, at 50 kV and 20 ma.

Film transmissions for the diffraction spots were read on a transmission photometer for the levels having $n=0$, 1, 2, 3, 7, and 8. Intensities for the levels having $n=4$, 5, and 6, and for $hk0$ and $0kl$ levels were estimated visually by comparison with a standard spot strip of intensities. The photometer readings of transmission T were converted to densities D according to the relationship $D=\text{colog } T$. Corrections were then made for Lorentz and polarization factors to obtain the observed structure amplitudes. No correction was made for absorption effects, which are relatively minor for the Mo radiation used. The final number of non-equivalent data available for least-squares refinement was 4399 *hkl*, of which 2997 had $|F_o|>0$.

Refinement procedures. Initial atomic parameters, taken from the low albite structure (Ferguson *et al.*, 1958), were refined at first by successive electron-density projections taken on planes normal to the *a*, *b*, and *c* axes. The various possibilities for the location of boron in one or more of the tetrahedral sites were examined by appropriate structure-factor calculations. The boron appeared to be wholly ordered in site $T_1(0)$ and was held in this site throughout the least-squares refinement. The final results fully confirm this assignment.

When the three-dimensional data became available, least-squares analysis was carried out using the full matrix of the normal equations according to a program written for the Burroughs 220 digital computer by J. Marshek of the U. S. Geological Survey, and one of us (D.E.A.). Thirteen cycles of refinement were made with about 2750 *hkl* reflections taken from all levels except those with $k=4$, 5, and 6. The refinement and weighting procedures used are the same as those described in Clark *et al.* (1964). The scattering factors during this portion of the refinement were as follows: zero-valence values for sodium and oxygen, and quadruply ionized values for silicon (Berghuis *et al.*, 1955); zero-valence values for boron (Ibers, 1957). An unweighted R-factor of 0.11 was obtained at the end of the thirteen cycles of refinement for those terms with $|F_o|>0$.

At this stage of the refinement, the data for the *h*4*l*, *h*5*l*, and *h*6*l* levels became available and were added to the previous data. Three least-squares cycles with the entire set of 4399 data were carried out, and individual isotropic temperature factors were refined. Scale factors were refined for each level. The same scattering factors as in the earlier refinement were used for oxygen and boron. Changes were made for sodium to singly ionized values and for silicon to triply ionized values, both from Table 3.31A, Int. Tables, Vol. III (1962). The R-factor increased to 0.17 when the additional data were added, but after the last three cycles of refinement R returned to 0.109 for the 2997 terms with $|F_o|>0$. The standard error in the observed structure factors is 3.12.

TABLE 3. ATOMIC PARAMETERS COMPARED FOR REEDMERGNERITE, $NaBSi_3O_8$, AND LOW ALBITE, $NaAlSi_3O_8$

Atom[1]	Low albite, $NaAlSi_3O_8$; Ribbe, Ferguson and Taylor (1962)			Reedmergnerite, $NaBSi_3O_8$ Present study[2]			
	Parameter (cycles)			Parameter (cycles)			B(Å^2)
	x	y	z	x	y	z	
$O_A(1)$	0.0057	0.1307	0.9669	0.0076	0.1364	1.0040	0.56
$O_A(2)$	0.5923	0.9972	0.2801	0.5929	0.9812	0.2758	0.55
$O_B(0)$	0.8124	0.1102	0.1904	0.8455	0.0995	0.2126	0.70
$O_B(m)$	0.8205	0.8517	0.2585	0.8163	0.8347	0.2335	0.71
$O_C(0)$	0.0140	0.3032	0.2695	0.0064	0.2762	0.2725	0.66
$O_C(m)$	0.0239	0.6934	0.2292	0.0289	0.6799	0.2070	0.74
$O_D(0)$	0.2068	0.1086	0.3894	0.1900	0.1200	0.3815	0.66
$O_D(m)$	0.1838	0.8682	0.4352	0.1922	0.8682	0.4172	0.63
$T_1(0)$	0.0087	0.1695	0.2083	0.0127	0.1617	0.2217	0.38
$T_1(m)$	0.0044	0.8203	0.2378	0.0059	0.8100	0.2097	0.28
$T_2(0)$	0.6919	0.1103	0.3148	0.7029	0.1015	0.3204	0.31
$T_2(m)$	0.6814	0.8819	0.3605	0.6847	0.8644	0.3547	0.31
$Na_1(0)$	0.2715	0.9779	0.1613	0.2586	1.0075	0.1332	1.22
Na_2	0.2651	0.9993	0.1310				

[1] Type atoms selected by Megaw (1956).

[2] Final parameters at end of 16 cycles of least-squares refinement; residual 0.109 for 2997 *hkl* with $|F_o|>0$. Standard errors as follows: oxygen atoms, $x, y, z\pm0.0004$, $B\pm0.03$ Å^2; boron atom in site $T_1(0)$, $x, y, z\pm0.0006$, $B\pm0.04$ Å^2; silicon atoms, $x, y, z\pm0.0002$, $B\pm0.01$ Å^2; sodium atom, $x, y, z\pm0.0003$, $B\pm0.03$ Å^2.

Atomic parameters, structure factors, and bond distances. The atomic parameters obtained from the refinement are listed in Table 3, together with the atomic parameters for low albite obtained after three-dimensional difference-synthesis refinement by Ribbe, Ferguson and Taylor (1962). Observed and calculated structure factors for reedmergnerite are given in Table 4.[1] At the completion of least-squares refinement, a three-dimensional difference synthesis was computed. Its generally featureless appearance (maximum values ±0.6 e/Å^3) confirms the results of the least-squares refinement.

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[1] Table 4 has been deposited as Document No. 8618 with the ADI Auxiliary Publications Project, Photoduplication Service, Library of Congress, Washington 25, D. C. A copy may be secured by citing the Document number and by remitting $12.50 for photoprints or $4.25 for 35 mm microfilm. Advance payment is required. Make checks or money orders payable to: Chief, Photoduplication Service, Library of Congress.

The bond distances and angles (Tables 5–8) were calculated from the atomic positions listed in Table 3, using the cell parameters given in Table 1. The calculations were carried out on the Burroughs 220 digital computer with programs written by D. S. Handwerker of the U. S. Geological Survey, and described in Clark *et al.* (1964). Bond distances and angles for low albite were calculated from the atomic parameters given by Ribbe, *et al.* (1962).

DESCRIPTION OF STRUCTURE

The feldspar crystal structure was established for sanidine by Taylor (1933) and for low albite by Taylor *et al.* (1934). Since that time a num-

TABLE 5. COMPARISON OF BOND DISTANCES FOR THE TETRAHEDRA OF REEDMERGNERITE $NaBSi_3O_8$, AND LOW ALBITE, $NaAlSi_3O_8$

Tetrahedron[1]	Oxygen Atom	Coordinates of Oxygen Atom	T-O Distance (Å)	
			Reedmergnerite	Low Albite[2]
(*a*) T-O Distances				
$T_1(0000)$	$O_A(1000)$	$x, y, z-1$	1.478±0.005	1.751
	$O_B(0000)$	$x-1, y, z$	1.470±0.006	1.745
	$O_C(0000)$	x, y, z	1.443±0.009	1.730
	$O_D(0000)$	x, y, z	1.467±0.006	1.751
		Average	*1.465*	*1.744*
$T_1(m000)$	$O_A(100c)$	$\bar{x}, 1-y, 1-z$	1.595±0.004	1.604
	$O_B(m000)$	$x-1, y, z$	1.602±0.003	1.601
	$O_C(m000)$	x, y, z	1.624±0.005	1.623
	$O_D(m000)$	x, y, z	1.618±0.003	1.612
		Average	*1.610*	*1.610*
$T_2(0000)$	$O_A(2000)$	$x, y-1, z$	1.634±0.005	1.635
	$O_B(0000)$	x, y, z	1.585±0.003	1.592
	$O_C(m0i0)$	$1/2+x, y-1/2, z$	1.625±0.005	1.614
	$O_D(m00c)$	$1-x, 1-y, 1-z$	1.613±0.003	1.621
		Average	*1.614*	*1.616*
$T_2(m000)$	$O_A(2000)$	x, y, z	1.646±0.005	1.643
	$O_B(m000)$	x, y, z	1.620±0.003	1.620
	$O_C(00i0)$	$1/2+x, 1/2+y, z$	1.606±0.004	1.585
	$O_D(000c)$	$1-x, 1-y, 1-z$	1.614±0.003	1.602
		Average	*1.622*	*1.613*

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[1] Site $T_1(0)$ occupied by B in reedmergnerite, Al in low albite; all other tetrahedral sites occupied by Si in both minerals.

[2] T-O distances from Ribbe *et al.* (1962); O-O distances calculated by present authors from atomic coordinates given by Ribbe *et al.* (1962).

TABLE 5—(*continued*)

Tetrahedron[1]	Oxygen Atom	Coordinates of Oxygen Atom	*T*-O Distance (Å)	
			Reedmergnerite	Low Albite[2]
(*b*) O-O Distances Within Tetrahedra				
$T_1(0)$	$O_A(1)$—$O_B(0)$		2.338±0.004	2.729
	$O_A(1)$—$O_C(0)$		2.444±0.006	2.953
	$O_A(1)$—$O_D(0)$		2.345±0.004	2.750
	$O_B(0)$—$O_C(0)$		2.402±0.007	2.897
	$O_B(0)$—$O_D(0)$		2.415±0.004	2.871
	$O_C(0)$—$O_D(0)$		2.401±0.007	2.862
		Average	*2.391*	*2.844*
$T_1(m)$	$O_A(1)$—$O_B(m)$		2.579±0.004	2.603
	$O_A(1)$—$O_C(m)$		2.712±0.007	2.687
	$O_A(1)$—$O_D(m)$		2.580±0.004	2.587
	$O_B(m)$—$O_C(m)$		2.631±0.006	2.618
	$O_B(m)$—$O_D(m)$		2.644±0.004	2.655
	$O_C(m)$—$O_D(m)$		2.622±0.007	2.625
		Average	*2.628*	*2.629*
$T_2(0)$	$O_A(2)$—$O_B(0)$		2.619±0.005	2.663
	$O_A(2)$—$O_C(m)$		2.552±0.007	2.565
	$O_A(2)$—$O_D(m)$		2.620±0.005	2.615
	$O_B(0)$—$O_C(m)$		2.690±0.005	2.656
	$O_B(0)$—$O_D(m)$		2.672±0.004	2.659
	$O_C(m)$—$O_D(m)$		2.640±0.004	2.659
		Average	*2.632*	*2.636*
$T_2(m)$	$O_A(2)$—$O_B(m)$		2.653±0.006	2.620
	$O_A(2)$—$O_C(0)$		2.595±0.007	2.574
	$O_A(2)$—$O_D(0)$		2.619±0.005	2.635
	$O_B(m)$—$O_C(0)$		2.637±0.004	2.631
	$O_B(m)$—$O_D(0)$		2.669±0.004	2.637
	$O_C(0)$—$O_D(0)$		2.703±0.005	2.688
		Average	*2.646*	*2.631*

ber of studies of various feldspar structures by members of the Cambridge school have appeared. Those that are particularly pertinent to the present discussion are the two-dimensional refinements of low and high albite by Ferguson, Traill and Taylor (1958), the three-dimensional refinements of low albite by Ribbe, *et al.* (1962), and of maximum microcline by Brown and Bailey (1964), and the extensive studies of anorthite by Kempster, *et al.* (1962) and Megaw *et al.* (1962). A review paper on the structures of the principal feldspars by Taylor (1962) is also valuable.

Since reedmergnerite is isostructural with low albite, the existing comprehensive literature makes discussion of the general structural features unnecessary. Instead, we will compare structural details between reedmergnerite and low albite in particular, extending the comparison to include other feldspars as warranted. The standard notation of Megaw (1956) has been used throughout the discussion, in the current form that designates tetrahedral cation sites impartially as *T*. A view of the reedmergnerite structure with the type atoms identified is shown in Fig. 1.

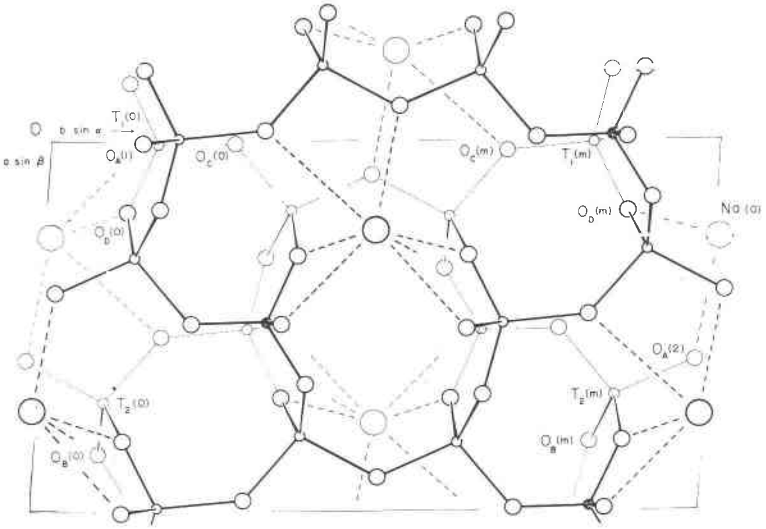

FIG. 1. View along *c* of the reedmergnerite structure with type atoms labelled. The boron atoms in site $T_1(0)$ are shaded, other *T* sites contain Si. Dashed lines indicate Na-O bonds.

The T-O tetrahedra. Comparison of *T*-O and O-O distances are made in Table 5 for reedmergnerite and low albite. The O-*T*-O angles are compared in Table 6. Since reedmergnerite contains no tetrahedrally coordinated cation larger than Si, substitution, were it to occur, would result in decreasing rather than increasing the observed *T*-O distance. However, not only the average values, but almost all the individual values, are so nearly alike in the $T_1(m)$, $T_2(0)$, and $T_2(m)$ sites of both minerals that there can be little doubt the tetrahedral cation in each site is Si. The site $T_1(0)$ is therefore wholly ordered in each mineral, containing the boron in reedmergnerite and the aluminum in low albite within the narrow limits of experimental error. An Al-occupancy figure of 0.93 for site $T_1(0)$ of low albite is obtained from Smith's revised relationship (Smith and Bailey, 1963) for determination of Al-content from average

TABLE 6. COMPARISON OF BOND ANGLES FOR THE TETRAHEDRA OF REEDMERGNERITE, $NaBSi_3O_8$, AND LOW ALBITE, $NaAlSi_3O_8$

Tetrahedron[1]	Atoms[2]	Angle	
		Reedmergnerite	Low Albite[3]
$T_1(0)$	$O_A(1)$—T—$O_B(0)$	104°56′±22′	102°40′
	$O_A(1)$—T—$O_C(0)$	113°27′±29′	116°04′
	$O_A(1)$—T—$O_D(0)$	105°34′±22′	103°32′
	$O_B(0)$—T—$O_C(0)$	110°57′±22′	112°58′
	$O_B(0)$—T—$O_D(0)$	110°37′±29′	110°24′
	$O_C(0)$—T—$O_D(0)$	111°03′±22′	110°36′
$T_1(m)$	$O_A(1)$—Si—$O_B(m)$	107°34′±15′	108°37′
	$O_A(1)$—Si—$O_C(m)$	114°48′±17′	112°43′
	$O_A(1)$—Si—$O_D(m)$	106°50′±16′	107°06′
	$O_B(m)$—Si—$O_C(m)$	109°16′±18′	108°35′
	$O_B(m)$—Si—$O_D(m)$	110°23′±14′	111°27′
	$O_C(m)$—Si—$O_D(m)$	107°56′±14′	108°25′
$T_2(0)$	$O_A(2)$—Si—$O_B(0)$	108°52′±17′	111°12′
	$O_A(2)$—Si—$O_C(m)$	103°08′±13′	104°19′
	$O_A(2)$—Si—$O_D(m)$	107°38′±14′	106°53′
	$O_B(0)$—Si—$O_C(m)$	113°52′±17′	111°54′
	$O_B(0)$—Si—$O_D(m)$	113°22′±12′	111°40′
	$O_C(m)$—Si—$O_D(m)$	109°18′±16′	110°32′
$T_2(m)$	$O_A(2)$—Si—$O_B(m)$	108°37′±15′	106°51′
	$O_A(2)$—Si—$O_C(0)$	105°53′±12′	105°45′
	$O_A(2)$—Si—$O_D(0)$	106°55′±16′	108°35′
	$O_B(m)$—Si—$O_C(0)$	109°40′±17′	110°21′
	$O_B(m)$—Si—$O_D(0)$	111°16′±12′	109°53′
	$O_C(0)$—Si—$O_D(0)$	114°10′±15′	115°02′

[1] Site $T_1(0)$ occupied by B in reedmergnerite, Al in low albite; all other tetrahedral sites occupied by Si in both minerals.

[2] Coordinates of atoms as in Table 5 (*a*).

[3] Angles calculated by present authors from atomic coordinates given by Ribbe *et al.* (1962).

T-O distance. This figure must simply indicate the magnitude of the errors involved in such estimations. These errors are apparently closer to ±8% than to the ±5% (in round figures) proposed by Smith and Bailey (1963). In maximum microcline (Brown and Bailey, 1964), a 0.94 Al-occupancy factor for site $T_1(0)$ obtained from Smith's revised relationship was used as partial evidence for deviation from perfect order. Since this "occupancy factor" is so close to that found for low albite, its merit as evidence for disorder is doubtful.

It is noteworthy that the feldspar framework can accommodate to either the shorter B-O distances (average value, 1.465 Å) or the longer Al-O distances (average value, 1.744 Å) without significantly altering the dimensions of the Si-O tetrahedra. The effects of the substitution appear to be distributed over the entire cell, principally as changes in T-O-T angles. These changes, together with the smaller size of the B-O tetrahedra, result in the smaller unit-cell dimensions found for reedmergnerite (Table 1). The B-O distances, O-B-O angles, and O-O distances in the borate tetrahedron of reedmergnerite are all in good agreement with those found for borate tetrahedra in numerous borate structures (*e.g.*, in the refinement of five calcium borates, Clark *et al.*, 1964).

The overall average Si-O distance is 1.615 Å in reedmergnerite and 1.613 Å in low albite. These values confirm the rounded-off value of 1.61 Å for the average Si-O distance in framework structures that was proposed by Smith and Bailey (1963). The range of Si-O values is almost identical for both minerals, *i.e.* from 1.646±0.005 Å to 1.585±0.003 Å in reedmergnerite, and from 1.643 Å to 1.585 Å in low albite. The same pair of atoms, $T_2(m)$-$O_A(2)$, is associated with the longest Si-O distances in both minerals. Comparison of like individual distances shows that only one pair, $T_2(m)$-$O_C(0)$, differs by more than 0.012 Å, and none of the like O-Si-O angles differs by more than 2°20′.

All the tetrahedral cations in reedmergnerite have isotropic temperature factors of about 0.3 Å^2 (Table 3); differences among the individual values are not significant. The oxygen atoms have an average isotropic temperature factor of 0.65 Å^2. These values are normal for an ordered structure (Burnham, 1964). Temperature factors are not currently available from the three-dimensional refinement of the low albite data, but the average isotropic temperature factors in anorthite (Kempster *et al.*, 1962) and in maximum microcline (Brown and Bailey, 1964) are comparable to those found for reedmergnerite, *i.e.* 0.2 to 0.4 Å^2 for the tetrahedral cations, and 0.6 to 1.0 Å^2 for the oxygen atoms.

Environment of Na. In reedmergnerite, Na is coordinated by five oxygen atoms within a range of 2.380±0.004 Å to 2.489±0.005 Å, the average distance being 2.426 Å (Table 7). Both the range and the average value are slightly higher than those given for fivefold oxygen coordination of Na in Int. Tables, Vol. III (1962). In addition to the five close oxygen atoms, there are two at somewhat longer distances: $O_C(m)$ at 2.808 ±0.005 Å and $O_D(m)$ at 2.860±0.005 Å. Other neighbors are distant by more than three Ångstroms. The closest Na-Na approach is 3.622 ±0.004 Å. Comparison with the Na coordination in low albite is hampered by the extreme anisotropy associated with the Na atom in that structure. Coordinates have been assigned by Ribbe *et al.* (1962) for two distinct positions said to be randomly occupied in albite by the Na atom. The Na-O bond distances for each of these positions are tabulated in Table 7 (calculated from coordinates given by Ribbe *et al.*). The unusual anisotropy of the Na atom persists in low albite even at −180° C. (Williams and Megaw, 1964). The O-O distances in the Na coordination polyhedron are compared for reedmergnerite and low albite in Table 8. The longest diagonals are 5.275±0.006 Å (reedmergnerite), compared to 5.736 Å (albite), and 5.854±0.006 Å (reedmergnerite) compared to 5.593 Å (albite). The somewhat smaller overall size of the Na coordination polyhedron in reedmergnerite (approximately 11% less volume than in albite) may account for the fixed location of the Na cation in the boron feldspar.

TABLE 7. Na-O ENVIRONMENT IN REEDMERGNERITE, $NaBSi_3O_8$, AND LOW ALBITE, $NaAlSi_3O_8$

Oxygen Atom[1]	Coordinates of Oxygen Atom	Na-O Distance (Å)		
		Reedmergnerite	Low Albite[2]	
			Na_1	Na_2
$O_A(1000)$	$x, y+1, z-1$	2.455±0.005	2.794	2.540
$O_A(100c)$	$x, 1-y, 1-z$	2.489±0.005	2.464	2.618
$O_A(2000)$	x, y, z	2.397±0.004	2.374	2.385
$O_B(000c)$	$1-x, 1-y, \bar{z}$	2.410±0.004	2.483	2.437
$O_B(m00c)$	$1-x, 2-y, z$	3.117±0.005	3.630	3.293
$O_C(00i0)$	$1/2+x, 1/2+y, z$	3.452±0.006	2.932	3.088
$O_C(m0i0)$	$1/2+x, 1/2+y, z$	2.808±0.005	3.379	3.152
$O_D(0000)$	$x, 1+y, z$	2.380±0.004	2.454	2.437
$O_D(m000)$	x, y, z	2.860±0.005	2.840	3.149

[1] Oxygen atoms coordinating Na(0000) at x, y, z (Table 3).

[2] Values calculated by present authors from atomic coordinates of Ribbe *et al.* (1962).

There are other points of difference betwen the Na coordination in reedmergnerite and low albite. First, one change occurs in the type atoms which coordinate the Na cation: $O_C(m)$ at 2.808±0.005 Å in reedmergnerite, but $O_C(0)$ at either 2.932 or 3.088 Å in low albite. The remainder of the Na coordination polyhedron consists of the same type atoms in both compounds. Second, there is no evidence from the reedmergnerite data for the presence of any anisotropic thermal motion associated with the Na cation. Its isotropic temperature factor is 1.22 ±0.03 Å^2, a reasonable value, which is comparable to the 1.41±0.03 Å^2

TABLE 8. O-O DISTANCES IN THE Na COORDINATION POLYHEDRON OF REEDMERGNERITE $NaBSi_3O_8$, AND OF LOW ALBITE, $NaAlSi_3O_8$

Oxygen Atoms[1]	Distance (Å)		Oxygen Atoms[1]	Distance (Å)	
	Reedmergnerite	Low Albite[2]		Reedmergnerite	Low Albite[2]
$O_A(100c)$-$O_B(0)$	2.338±0.004	2.729	$O_A(100c)$-$O_C(0)$	3.839±0.004	3.871
$O_A(1000)$-$O_D(0)$	2.345±0.004	2.750	$O_A(2)$-$O_D(m)$	3.905±0.004	4.363
$O_A(2)$-$O_C(m)$	2.552±0.007	2.565	$O_A(2)$-$O_D(0)$	3.960±0.005	3.761
$O_A(100c)$-$O_D(m)$	2.580±0.004	2.587	$O_B(0)$-$O_D(m)$	4.206±0.004	4.520
$O_A(2)$-$O_C(0)$	2.595±0.007	2.574	$O_A(1000)$-$O_D(m)$	4.335±0.006	4.643
$O_D(0)$-$O_D(m)$	3.136±0.007	3.138	$O_A(100c)$-$O_A(2)$	4.370±0.004	4.691
$O_C(0)$-$O_D(m)$	3.247±0.005	3.440	$O_B(0)$-$O_C(m)$	4.402±0.006	4.831
$O_A(1000)$-$O_A(100c)$	3.366±0.010	3.422	$O_B(0)$-$O_D(0)$	4.632±0.005	4.772
$O_C(m)$-$O_D(0)$	3.430±0.004	3.495	$O_A(1000)$-$O_A(2)$	4.651±0.005	4.590
$O_A(2)$-$O_B(0)$	3.615±0.004	3.718	$O_C(0)$-$O_C(m)$	5.039±0.008	5.026
$O_A(1000)$-$O_B(0)$	3.639±0.006	3.680	$O_C(0)$-$O_D(0)$	5.174±0.007	4.780
$O_A(1000)$-$O_C(m)$	3.690±0.004	3.863	$O_C(m)$-$O_D(m)$	5.205±0.006	5.714
$O_B(0)$-$O_C(0)$	3.696±0.005	3.406	$O_A(100c)$-$O_C(m)$	5.275±0.006	5.736
$O_A(100c)$-$O_D(0)$	3.795±0.006	3.764	$O_A(1000)$-$O_C(0)$	5.854±0.006	5.593

[1] Coordinates as given in Table 7; Na atom coordinated by $O_C(0)$ in low albite, $O_C(m)$ in reedmergnerite. All other coordinating oxygen atoms are the same in both structures.

[2] Values calculated by present authors from atomic coordinates given by Ribbe *et al.* (1962).

TABLE 9. COMPARISON OF DISTANCES FOR THE FOUR-MEMBERED RINGS OF REEDMERGNERITE, $NaBSi_3O_8$, AND LOW ALBITE, $NaAlSi_3O_8$

(*a*) Ring 1 (Fig. 2) Atom	Coordinates	Atom	Coordinates
$T_1(0000)$	x, y, z	$T_1(00ic)$	$1/2-x,\ 1/2-y,\ 1-z$
$O_D(0000)$	x, y, z	$O_D(00ic)$	$1/2-x,\ 1/2-y,\ 1-z$
$T_2(m00c)$	$1-x,\ 1-y,\ 1-z$	$T_2(m0i0)$	$x-1/2,\ y-1/2,\ z$
$O_C(00ic)$	$1/2-x,\ 1/2-y,\ 1-z$	$O_C(0000)$	x, y, z

Atoms	Distance[1] (Å)		Atoms	Angle	
	Reedmergnerite	Low Albite[2]		Reedmergnerite	Low Albite[2]
$T_1(0)$-$O_D(0)$	1.467±0.006	1.751	$T_1(0)$-$O_D(0)$-$T_2(m)$	135°22′±20′	133°57′
$O_D(0)$-$T_2(m)$	1.614±0.003	1.602	$O_D(0)$-$T_2(m)$-$O_C(0)$	114°10′±15′	115°02′
$T_2(m)$-$O_C(0)$	1.606±0.004	1.585	$T_2(m)$-$O_C(0)$-$T_1(0)$	124°56′±16′	130°04′
$O_C(0)$-$T_1(0)$	1.445±0.009	1.730	$O_C(0)$-$T_1(0)$-$O_D(0)$	111°03′±22′	110°36′
$T_1(0000)$-$T_2(m00c)$	2.850±0.004	3.086			
$T_1(0000)$-$T_2(m0i0)$	2.706±0.007	3.006			
$T_1(0000)$-$T_1(00ic)$	4.346±0.009	4.668			
$T_2(m00c)$-$T_2(m0i0)$	3.465±0.004	3.915			
$O_C(0000)$-$O_C(00ic)$	3.806±0.006	4.050			
$O_D(0000)$-$O_D(00ic)$	3.413±0.010	3.798			

[1] T-O and O-O distances not listed here are given in Table 5.

[2] Values calculated by present authors from atomic coordinates given by Ribbe *et al.* (1962).

TABLE 9—(*continued*)

(*b*) Ring 2 (Fig. 2) Atom	Coordinates	Atom	Coordinates
$T_1(m000)$	$x, y,$	$T_1(m0ic)$	$1/2-x, 3/2-y, 1-z$
$O_D(m000)$	x, y, z	$O_D(m0ic)$	$1/2-x, 3/2-y, 1-z$
$T_2(000c)$	$1-\boldsymbol{x}, 1-y, 1-z$	$T_2(00i0)$	$x-1/2, 1/2+y, z$
$O_C(m0ic)$	$1/2-x, 3/2-y, 1-z$	$O_C(m000)$	x, y, z

Atoms	Distance (Å)		Atoms	Angle	
	Reedmergnerite	Low Albite[2]		Reedmergnerite	Low Albite[2]
$T_1(m)$-$O_D(m)$	1.618 ± 0.003	1.612	$T_1(m)$-$O_D(m)$-$T_2(0)$	146°20′± 13′	151°22′
$O_D(m)$-$T_2(0)$	1.613 ± 0.003	1.621	$O_D(m)$-$T_2(0)$-$O_C(m)$	109°18′± 16′	110°32′
$T_2(0)$-$O_C(m)$	1.625 ± 0.005	1.614	$T_2(0)$-$O_C(m)$-$T_1(m)$	135°53′± 15′	135°34′
$O_C(m)$-$T_1(m)$	1.624 ± 0.005	1.623	$O_C(m)$-$T_1(m)$-$O_D(m)$	107°56′± 14′	108°25′
$T_1(m000)$-$T_2(000c)$	3.092 ± 0.002	3.134			
$T_1(m000)$-$T_2(00i0)$	3.011 ± 0.003	2.997			
$T_1(m000)$-$T_1(m0ic)$	4.483 ± 0.002	4.506			
$T_2(000c)$-$T_2(00i0)$	4.142 ± 0.003	4.158			
$O_C(m000)$-$O_C(m0ic)$	4.172 ± 0.006	4.182			
$O_D(m000)$-$O_D(m0ic)$	3.208 ± 0.010	3.229			

(*c*) Ring 3 (Fig. 4) Atom	Coordinates	Atom	Coordinates
$T_1(m0i0)$	$1/2+x, y-1/2, z$	$T_1(00ic)$	$1/2-x, 1/2-y, 1-z$
$O_B(m0i0)$	$x-1/2, y-1/2, z$	$O_B(00ic)$	$3/2-x, 1/2-y, 1-z$
$T_2(m0i0)$	$x-1/2, y-1/2, z$	$T_2(00ic)$	$3/2-x, 1/2-y, 1-z$
$O_D(00ic)$	$1/2-x, 1/2-y, 1-z$	$O_D(m0i0)$	$1/2+x, y-1/2, z$

Atoms	Distance[1] (Å)		Atoms	Angle	
	Reedmergnerite	Low Albite[2]		Reedmergnerite	Low Albite[2]
$T_1(m)$-$T_2(m)$	3.163 ± 0.002	3.177	$T_1(m)$-$O_B(m)$-$T_2(m)$	158°05′± 12′	161°00′
$T_1(m)$-$T_1(0)$	3.931 ± 0.004	4.005	$O_B(m)$-$T_2(m)$-$O_D(0)$	111°16′± 12′	109°53′
$T_1(m)$-$T_2(0)$	3.092 ± 0.002	3.134	$T_2(m)$-$O_D(0)$-$T_1(0)$	135°22′± 20′	133°57′
$T_2(m)$-$T_1(0)$	2.850 ± 0.004	3.086	$O_D(0)$-$T_1(0)$-$O_B(0)$	110°37′± 29′	110°24′
$T_2(m)$-$T_2(0)$	4.290 ± 0.002	4.564	$T_1(0)$-$O_B(0)$-$T_2(0)$	140°28′± 23′	139°31′
$T_1(0)$-$T_2(0)$	2.875 ± 0.004	3.131	$O_B(0)$-$T_2(0)$-$O_D(m)$	113°22′± 12′	111°40′
$O_B(m)$-$O_B(0)$	3.537 ± 0.004	3.742	$T_2(0)$-$O_D(m)$-$T_1(m)$	146°20′± 13′	151°22′
$O_D(0)$-$O_D(m)$	3.809 ± 0.004	3.899	$O_D(m)$-$T_1(m)$-$O_B(m)$	110°23′± 14′	111°27′

isotropic value found for the K cation in maximum microcline (Brown and Bailey, 1964). The final three-dimensional difference synthesis for reedmergnerite shows no pronounced peaks or troughs in the vicinity of the Na location. This result suggests that the observed anisotropy in low albite is due to a space-average effect, rather than a time-average effect, and that the Na cation in fact occupies only one of the distinct positions in any one cell. Both possibilities have been discussed by Ferguson *et al.* (1958). The question has been raised by Williams and Megaw (1964) as to whether the "half-atom" splitting of the Na atoms in low albite is due to "statistical occupation of two sites or to an ordered alteration within small domains." The difference between these two models does not appear to be significant, since the domain size is too small to affect the diffraction patterns.

FELDSPAR STRUCTURAL FEATURES

The framework of linked tetrahedra. The concept of the feldspar structure as a (Si, Al)-O framework constructed from elastic "building elements" was introduced by Megaw *et al.* (1962) in their discussion of the anorthite structure. The authors point out that rigid, regular tetrahedra probably could not be linked together to produce the feldspar framework, so some flexibility must be associated with the "building elements." The deviations from regularity are called strains by Megaw *et al.* and are tabulated in their Table 10 for like oxygen atoms in seven different feldspar structures. The remarkable similarities in magnitude and direction of the deviations from regularity in all the structures are conclusively demonstrated and lend support to the idea that the deviations are inherent in the structure of the framework.

TABLE 10. COMPARISON OF BOND DISTANCES AND ANGLES ASSOCIATED WITH THE O_A OXYGEN ATOMS IN REEDMERGNERITE, $NaBSi_3O_8$, AND LOW ALBITE, $NaAlSi_3O_8$

Atoms	Distance (Å)		Atoms	Angle	
	Reedmergnerite	Low Albite[1]		Reedmergnerite	Low Albite[1]
$O_A(1)$-$T_1(0)$	1.478±0.005	1.751	$T_1(0)$-$O_A(1)$-$T_1(m)$	143°05′±29′	140°37′
$O_A(1)$-$T_1(m)$	1.595±0.004	1.604	$T_2(0)$-$O_A(2)$-$T_2(m)$	128°40′±10′	130°11′
$O_A(2)$-$T_2(0)$	1.634±0.004	1.635			
$O_A(2)$-$T_2(m)$	1.646±0.005	1.643			
$T_1(0)$-$T_1(m)$	2.915±0.004	3.159			
$T_2(0)$-$T_2(m)$	2.956±0.003	2.973			

[1] Values calculated by present authors from atomic coordinates given by Ribbe *et al.* (1962).

We have made similar calculations for reedmergnerite and for the new values of low albite (Ribbe *et al.*, 1962), and the results for the silicate tetrahedra in these two structures are compared with those for maximum microcline (Brown and Bailey, 1964) and anorthite in Table 11. The maximum deviations are approximately ±0.1 Å for the O-O tetrahedral edges and approximately ±6° for the O-Si-O angles. The limits of flexibility thus appear to be well defined. In all four structures the largest deviations, both greater and smaller than the values for regular tetrahedra, are associated with a combination of type A and C oxygen atoms.

A comparison of the deviations from regularity of the various $T_1(0)$

TABLE 11. COMPARISON OF DEVIATIONS FROM REGULARITY OF O-O TETRAHEDRON EDGES AND O-Si-O BOND ANGLES IN Si-O TETRAHEDRA OF REEDMERGNERITE, $NaBSi_3O_8$, LOW ALBITE, $NaAlSi_3O_8$, MAXIMUM MICROCLINE, $KAlSi_3O_8$, AND ANORTHITE, $CaAl_2Si_2O_8$

Oxygen Atoms of Edge	Tetrahedron	Difference of O-O Edge from Ideal Value[1] (2.640 Å)				Difference of O-Si-O Angles from Ideal Tetrahedral Angle[1] (109°28′)			
		Reedmergnerite	Low Albite	Maximum Microcline	Anorthite	Reedmergnerite	Low Albite	Maximum Microcline	Anorthite
		Present Study	Ribbe *et al.* (1962)	Brown and Bailey (1964)	Megaw *et al.* (1962)	Present Study	Ribbe *et al.* (1962)	Brown and Bailey (1964)	Megaw *et al.* (1962)
AB	$T_1(m)$	−0.061	−0.037	−0.049	−0.098	−1°54′	−0°51′	−1°21′	−6°18′
	$T_2(0)$	−0.021	+0.023	−0.002	−0.029	−0°36′	+1°44′	+2°14′	−1°54′
	$T_2(m)$	+0.013	−0.020	−0.034	+0.019	−0°51′	−2°37′	−3°20′	+1°18′
AC	$T_1(m)$	+0.072	+0.047	+0.040	+0.086	+5°20′	+3°15′	+3°43′	+4°30′
	$T_2(0)$	−0.088	−0.075	−0.084	−0.120	−6°20′	−5°09′	−5°38′	−7°18′
	$T_2(m)$	−0.045	−0.066	−0.078	−0.059	−3°35′	−3°43′	−4°48′	−4°30′
AD	$T_1(m)$	−0.060	−0.053	−0.042	−0.089	−2°38′	−2°22′	−1°52′	−4°54′
	$T_2(0)$	−0.020	−0.025	−0.027	+0.007	−1°50′	−2°35′	−1°43′	+1°54′
	$T_2(m)$	−0.021	−0.005	−0.002	+0.016	−2°33′	−0°53′	−0°12′	−0°12′
BC	$T_1(m)$	−0.009	−0.022	−0.008	+0.041	−0°12′	−0°53′	−0°43′	+2°30′
	$T_2(0)$	+0.050	+0.016	+0.008	+0.054	+4°24′	+2°26′	+1°49′	+2°48′
	$T_2(m)$	−0.003	−0.009	−0.009	+0.014	+0°12′	+0°53′	+0°38′	+2°18′
BD	$T_1(m)$	+0.004	+0.015	+0.027	+0.056	+0°55′	+1°59′	+1°32′	+4°24′
	$T_2(0)$	+0.032	+0.019	+0.008	−0.036	+3°54′	+2°12′	+2°29′	−0°54′
	$T_2(m)$	+0.029	−0.003	+0.007	−0.041	+1°48′	+0°25′	+1°44′	−1°18′
CD	$T_1(m)$	−0.018	−0.015	−0.002	−0.017	−1°32′	−1°03′	−1°16′	−0°42′
	$T_2(0)$	0	+0.019	+0.025	+0.060	−0°10′	+1°04′	+0°28′	+4°54′
	$T_2(m)$	+0.063	+0.048	+0.044	+0.032	+4°42′	+5°34′	+5°26′	+2°18′
Average		±0.034	±0.029	±0.028	±0.048	±2°24′	±2°12′	±2°16′	±3°03′

[1] Assuming a regular tetrahedron with Si-O distances of 1.614 Å (Megaw *et al.*, 1962). For reedmergnerite the associated errors are as in Table 5 (O-O) and Table (O-Si-O). For low albite, maximum microcline, and anorthite, the values are those obtained by the present authors using data from the respective sources. For anorthite an average of two independent values for O-O and O-Si-O, given in Table 2 (d) and (f) (Megaw *et al.*, 1962), was taken.

tetrahedra (Table 12)—B-O in reedmergnerite, Al-O in low albite, maximum microcline, and anorthite—shows a somewhat smaller range of deviations, ±0.06 Å, for the O-O edges of the B-O tetrahedron compared with those of the Al-O tetrahedra, especially in anorthite, in which the range is ±0.20 Å. The trend is not as definite for the angular deviations, but the largest ones are associated with the O-$Al_1(0)$-O angles of anorthite. Comparison of the remaining Al-O tetrahedra, $T_1(m)$, $T_2(0)$, and

$T_2(m)$, in anorthite with the corresponding Si-O tetrahedra in all four structures shows the following ranges of deviation. For the O-O edges in Si-O tetrahedra, -0.084 to $+0.072$ Å (average, ± 0.03 Å), for all except anorthite, which has a slightly larger range, -0.120 to $+0.086$ Å (average, ± 0.05 Å). In the Al-O tetrahedra of anorthite, a significant increase from these values occurs, -0.181 to $+0.120$ Å (average ± 0.064 Å). For the O-Si-O angles, a range of -7.3 to $+5.4°$ (average, $\pm 3°$) represents the limits of deviations for all four structures, whereas the comparable O-Al-O angles in anorthite deviate by a range of -8.1 to $6.5°$ (average, $\pm 4°$). These results suggest that Al-O tetrahedra tend to deviate more from regularity than either B-O or Si-O tetrahedra, possibly because of the longer Al-O distances and the resultant weakening of internal attractive forces. In the structure of sillimanite, Burnham (1963) also found the Al-O tetrahedra to be less regular than the Si-O tetrahedra.

Table 12. Comparison of Deviations from Regularity of O-O Tetrahedral Edges and O-*T*-O Bond Angles in the $T_1(0)$ Tetrahedra of Reedmergnerite, NaBSi$_3$O$_8$, Low Albite, NaAlSi$_3$O$_8$, Maximum Microcline, KAlSi$_3$O$_8$, and Anorthite, CaAl$_2$Si$_2$O$_8$

Oxygen Atoms of Edge	Difference of O-O Edge from Ideal Values[1]				Difference of O-*T*-O Angles from Ideal Tetrahedral Value (109°28′)			
	Reedmergnerite	Low Albite	Maximum Microcline	Anorthite	Reedmergnerite	Low Albite	Maximum Microcline	Anorthite
	Present Study	Ribbe *et al.* (1962)	Brown and Bailey (1964)	Megaw *et al.* (1962)	Present Study	Ribbe *et al.* (1962)	Brown and Bailey (1964)	Megaw *et al.* (1962)
AB	−0.062	−0.131	−0.099	−0.200	−4°31′	−6°48′	−4°19′	−11°42′
AC	+0.044	+0.093	+0.050	+0.156	+3°59′	+6°36′	+3°53′	+10°12′
AD	−0.055	−0.110	−0.090	−0.179	−3°54′	−5°56′	−3°55′	−11°42′
BC	+0.002	+0.037	+0.040	+0.008	+1°29′	+3°30′	+3°14′	+3°06′
BD	+0.015	+0.011	+0.003	+0.129	+1°09′	+0°56′	+1°16′	+6°48′
CD	+0.001	+0.002	−0.021	+0.018	+1°35′	+1°58′	−0°23′	+2°06′
Average	±0.030	±0.064	±0.048	±0.115	±2°46′	±4°18′	±2°50′	±7°36′

In anorthite, Megaw *et al.* (1962) note an increase in average *T*-O distance with increase in the number of Ca neighbors associated with the oxygen atoms. In maximum microcline, Brown and Bailey (1964), observe an exactly opposite trend, the average *T*-O distance decreasing as the number of K neighbors increases. No clear correlation occurs in

[1] Assuming regular tetrahedra with B-O distance 1.470 Å, ideal O-O 2.400 Å (reedmergnerite); Al-O 1.749 Å, ideal O-O 2.860 Å (Al tetrahedron taken by Megaw *et al.*, 1962). For reedmergnerite, associated errors as in Table 5 (O-O) and Table 6 (O-*T*-O). Values for low albite, maximum microcline, and anorthite are those obtained by present authors using data from the respective sources. For anorthite an average of two independent O-O and O-*T*-O values from Table 2 (d) and (f) (Megaw *et al.*, 1962) was used.

either reedmergnerite or low albite. The single Si-O distances to the oxygen atom $O_A(1)$ which has two Na neighbors are shorter than the average Si-O distances for the oxygen atoms with only one or no Na neighbors, as in microcline; but the Al-O distances in low albite and the B-O distances in reedmergnerite are largest for the $O_A(1)$, as in anorthite. The possibility exists that the correlations observed in anorthite and microcline are fortuitous, but further experimental evidence from other structures is necessary to clarify this point.

Closed rings in the structure. The feldspar structure contains various closed rings, which are commonly referred to in terms of the number of tetrahedra linking at corners to form the rings (Smith and Rinaldi, 1962). The total number of atoms in a ring is twice the number of tetrahedra involved. Using this terminology, four-membered, six-membered, and eight-membered rings can be found in the feldspar structure.

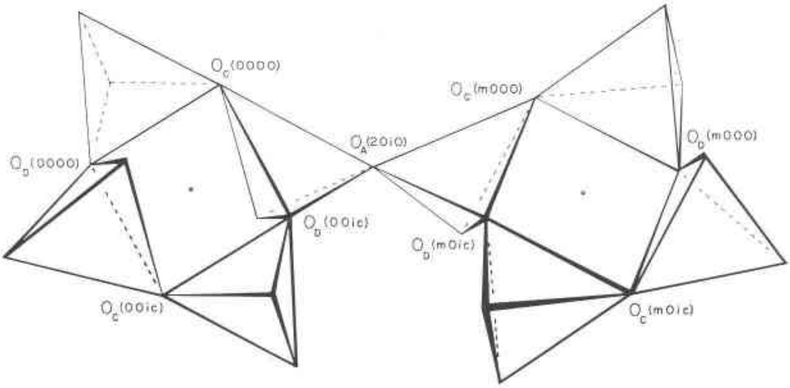

FIG. 2. Two four-membered rings in the reedmergnerite structure viewed along *c*; ring 1 on left, ring 2 on right. Symmetry centers are shown by small circles.

Three distinct four-membered rings are illustrated in Figs. 2 and 4 as they appear in reedmergnerite. Two of these rings (Nos. 1 and 2, Fig. 2) each have a center of symmetry, whereas the third ring (Fig. 4) does not. Some of the distances and angles are shown for rings 1 and 2 in Fig. 3 and for ring 3 in Fig. 5. The atomic coordinates for each ring and a complete list of pertinent distances and angles are given in Table 9 for both reedmergnerite and low albite. Examination of these values shows close agreement for most of the distances and angles in the two structures. Rings 1 and 2 are both considerably elongated along one diagonal, whereas ring 3 is more nearly equant.

A number of larger rings can be described, but all are constructed from

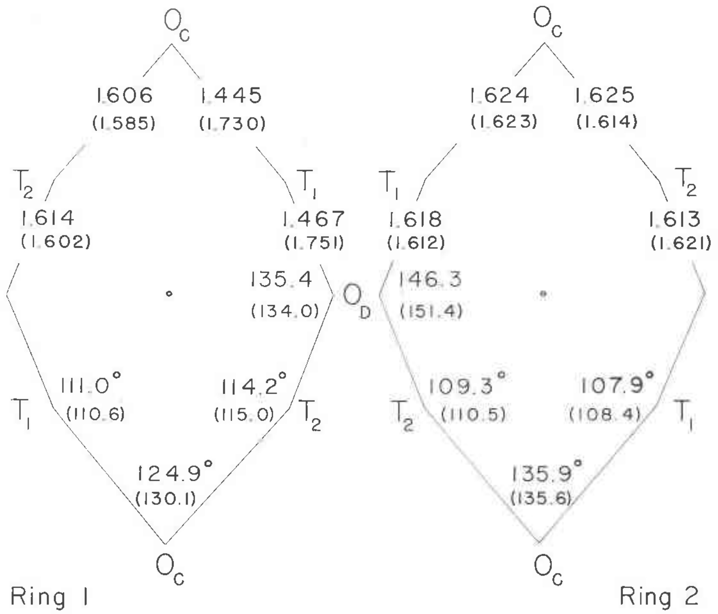

FIG. 3. Some distances (Å) and angles in the rings 1 and 2 shown in Fig. 2 (see also Table 9); values without parentheses are for reedmergnerite, with parentheses, for low albite.

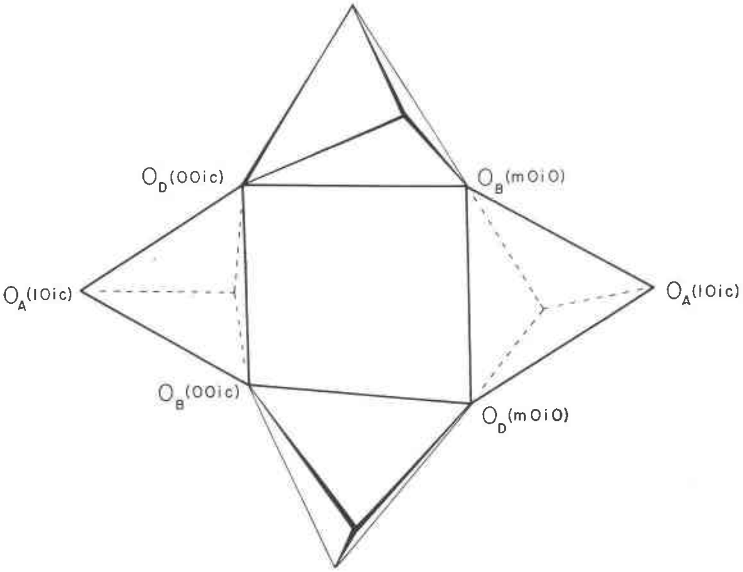

FIG. 4. Ring 3, a third four-membered ring in the reedmergnerite structure, viewed along *b*.

sections already shown for the four-membered rings combined with the two bridging sections associated with $O_A(1)$ and $O_A(2)$. The relevant distances and angles for the O_A oxygen atoms are given in Table 10.

Bond angles at oxygen atoms. These angles are compared in Table 13 for reedmergnerite, low albite, maximum microcline and anorthite. The overall similarities for like oxygen atoms are evident, as pointed out by Megaw *et al.* (1962) in their compilation for various feldspar structures. However, in some of these angles there are significant changes, which are apparently required by the framework in order to accommodate either boron or aluminum. The average values for anorthite are nearly all smaller than the corresponding values for the other two structures.

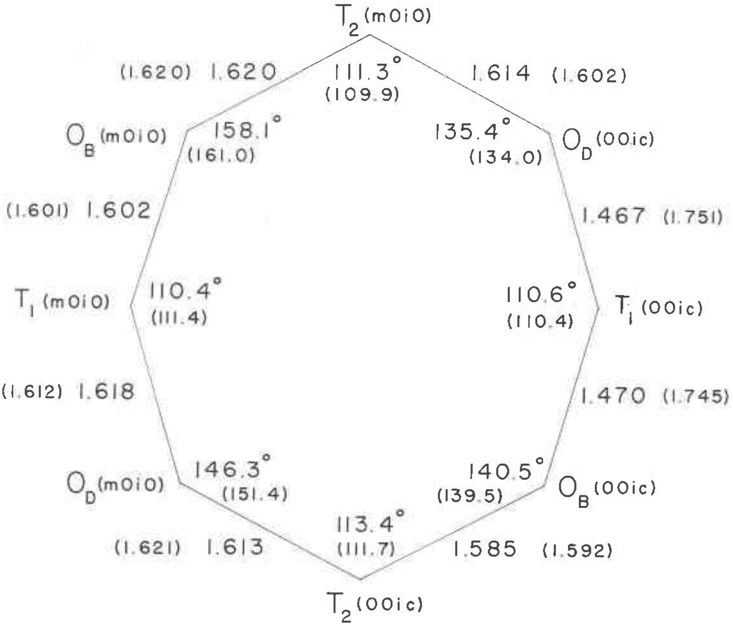

FIG. 5. Some distances (Å) and angles in the ring 3 shown in Fig. 4 (see also Table 9). Values without parentheses are for reedmergnerite; with parentheses, for low albite.

Charge balance in the feldspar structure. The complete refinement of the reedmergnerite structure does not significantly change either the values or the conclusions that have already been given on this subject (Clark and Appleman, 1960). We agree with Brown and Bailey (1964) that charge balance computations based on simple ionic models are not an adequate basis for evaluating the relative stabilities of different feldspar structures.

CONCLUSIONS

The present study underscores the similarities among the Si-O portions of the framework in chemically distinct feldspars. The striking correlation between Si-O distances for like atoms in reedmergnerite and low albite strongly indicates that both minerals are completely ordered and that the bond-distance values in maximum microcline (Brown and Bailey, 1964) cannot be used as evidence for partial disorder. The error associated with the use of Smith's relationship (as modified by Smith and Bailey, 1963) for Al-content as a function of average *T*-O bond distance is significantly larger than the ±5% (in round figures) suggested by those authors, and we suggest that a more realistic estimate of this error is ±8%. Accumulated evidence shows that Al-O tetrahedra in the feldspar framework deviate from regularity more than either Si-O or B-O tetrahedra. There is no anisotropy associated with the Na cation in reedmergnerite, a result that tends to confirm association of the observed anisotropy in low albite with a space-average effect, rather than a time-average effect.

TABLE 13. COMPARISON OF BOND ANGLES AT OXYGEN ATOMS FOR REEDMERGNERITE $NaBSi_3O_8$, LOW ALBITE, $NaAlSi_3O_8$, MAXIMUM MICROCLINE, $KAlSi_3O_8$, AND ANORTHITE, $CaAl_2Si_3O_8$

Oxygen Atom	Bond Angle, *T*-O-*T*				
	Reedmergnerite	Low Albite[1]	Maximum Microcline	Anorthite	
	Present Study	Ribbe *et al.* (1962)	Brown and Bailey (1964)	Megaw *et al.* (1962)	
				Average[2]	Range
$O_A(1)$	143.1±0.5°	140.6°	144.7°	136.9°	135–140°
$O_A(2)$	128.7±0.2°	130.2°	138.5°	124.4°	122–126°
$O_B(0)$	140.5±0.4°	139.5°	151.2°	133.3°	128–140°
$O_B(m)$	158.1±0.2°	161.0°	156.0°	155.8°	144–171°
$O_C(0)$	124.9±0.3°	130.0°	130.7°	131.4°	131–133°
$O_C(m)$	135.9±0.3°	135.6°	130.7°	129.8°	128–131°
$O_D(0)$	135.4±0.3°	134.0°	140.0°	130.0°	125–138°
$O_D(m)$	146.3±0.2°	151.5°	143.2°	151.8°	138-167°
Average	139.1°	140.3°	141.9°	136.7°	122–171°

[1] Values calculated by present authors from atomic coordinates of Ribbe *et al.* (1962).

[2] Average by present authors from values for four independent tetrahedra, Table 2 (g), Megaw *et al.* (1962).

Although reedmergnerite is so similar structurally to low albite, it has no disordered polymorph corresponding to high albite. This fact raises the possibility, first suggested by Prof. R. B. Ferguson (written comm., 1960), that although borosilicates can be synthesized which are exactly analogous to ordered aluminosilicates, it may be difficult or impossible for boron and silicon to occur in random occupancy of one atomic position in these structures. Thus there would be no borosilicate analogues of the disordered aluminosilicates. In this case the synthesis of borosilicate analogues, such as the various boron micas described by Eugster and Wright (1960), would provide a useful method for studying order-disorder problems in the corresponding aluminosilicates.

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