

## Bond Lengths in Alkali Felspars

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A study of the most accurate available measurements of bond lengths and contact distances in alkali felspars reveals interesting relationships with the degree of order of the Al,Si distribution in tetrahedral groups and throws light on the ionic character of the bonds between O and K or Na atoms.

### 1. Introduction

The potassium felspars ( $\text{KAlSi}_3\text{O}_8$ ) are more easily described than other felspars in terms of a simple model in which the relatively large potassium atom is in contact with 9 or 10 oxygen atoms forming the walls of a cavity within the framework of linked tetrahedral  $\text{SiO}_4$  and  $\text{AlO}_4$  groups. The mean T–O bond length for a given tetrahedron (T = Al or Si) is used as a measure of Al,Si occupancy, and the K–O contact distances cover a range of values in harmony with accepted ideas about atomic diameters.

In sodium felspars ( $\text{NaAlSi}_3\text{O}_8$ ) difficulties arise in considering the environment of the much smaller Na atom, which occupies the same structural cavity as is occupied by K though with some (relatively minor) changes in the (average) positions of the O atoms which form the cavity walls. For now the effective shape of the cation is no longer even approximately spherical (as in the potassium felspars) but is very elongated in one direction.

Even with the potassium felspars, however, the use of the simple model leads to difficulties when individual T–O bond lengths and K–O contact distances are studied in detail. From such studies there have developed the general ideas that the T–O bond may be partly covalent in character and that the length of the simple ionic K–O bond is subject to considerable modification, in different environments in the structure, under the influence of geometrical packing requirements.

Reedmergnerite ( $\text{NaBSi}_3\text{O}_8$ ), the boron analogue of (ordered) sodium felspar, while structurally very similar to low albite, shows differences in detail which have been discussed by Appleman & Clark (1965).

The need for further study is made clear by reference to two outstanding problems. First, in all felspars the contact K (or Na, Ca, Ba) to  $\text{O}_{A2}$  is abnormally short: in the ordered alkali felspars this means that a *short*, therefore on the most direct interpretation *strong*, bond O–K is provided by an O atom also linked to 2 Si by

tetrahedral bonds. Second, as pointed out by Brown & Bailey (1964), there is an apparent contradiction between the alkali felspars and anorthite in relation to the distribution of bonds. For in anorthite there is convincing evidence (Megaw, Kempster & Radoslovich, 1962) that the lengths of individual T–O bonds in this perfectly ordered structure are directly correlated with the numbers of bonds between O and Ca – very short (=strong) when the O atom is not coordinated to any Ca atom, progressively longer (=weaker) for O atoms coordinated to 1 or 2 Ca atoms. By contrast, in highly ordered microcline (Pellotsalo) Brown & Bailey (1964) found exactly the opposite variation in length of T–O bonds with variation in the number of contacts between O and K atoms.

In the present paper it is shown that it is possible to throw some light on the nature of the forces operative in the alkali felspars and to offer reasonably simple explanations of apparent anomalies in bond lengths and contact distances in these structures.

### 2. Bond lengths between K (or Na) and O in alkali felspars

The starting point for the discussion of the potassium felspars is the remark by Brown & Bailey (1964) that in maximum microcline (Pellotsalo), with nearly perfect Al,Si order, in the coordination polyhedron of O atoms around K 'the  $\text{O}_{A1}$  or  $\text{O}(0)$  atoms have excess negative charges and are correspondingly closer' (to K). The following developments of the implications of their statement, and the inclusion of the sodium felspars in a systematic scheme, rest on the most accurate measurements now available.

Sanidized orthoclase C (Spencer's notation) is conveniently taken to represent disordered potassium felspar, and in other materials the extent of the ordering is measured by the amount of Al in tetrahedral site  $\text{T}_1(0)$  into which all Al atoms are concentrated in the perfectly ordered structure. Then Table 1 shows that with increases in Al,Si order the distance K– $\text{O}_{A1}$  diminishes, distance K– $\text{O}_{A2}$  increases, while the *mean* distances from K to pairs of atoms  $\text{O}_B$ ,  $\text{O}_C$  and  $\text{O}_D$  remain essentially constant. This is in accordance with expectation since  $\text{O}_{A1}$  has  $\text{T}_1$  linkages only (and Al in

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$T_1$  increases as degree of order increases),  $O_{A2}$  has  $T_2$  linkages only (and Al in  $T_2$  decreases), while  $O_B$ ,  $O_C$  and  $O_D$  have linkages to both  $T_1$  and  $T_2$ . However, when *individual* distances from K to these atoms are examined (Table 2), an additional regularity with increasing order is at once apparent – bonds from K to  $O_B(0)$ ,  $O_C(0)$ ,  $O_D(0)$ , which in the fully ordered structure have T–O linkages (Al+Si) are shorter than in the disordered structure, whereas  $O_B(m)$ ,  $O_C(m)$  and  $O_D(m)$ , with linkages (Si+Si) are all longer.

To decide whether the sodium feldspars display similar trends is more complicated. First, there is no monoclinic (disordered) structure from which to measure changes in Na–O distances with change in order (as with monoclinic sanidine for K–O distances in the microclines); the best that can be done (Table 3) is to take the *mean* Na–O distances for (disordered) high albite for pairs of atoms  $O_{A1}(0)$  and  $O_{A1}(c)$ ,  $O_B(0)$  and  $O_B(m)$ , etc. with which to compare individual Na–O distances in the (ordered) low albite structure. Then again, it must not be forgotten that there is strong evidence (Ribbe, Megaw & Taylor, 1968) that half-atom or quarter-atom approximation is necessary for some

or all of the atoms in describing the structures of both high and low albites, whereas the distances listed in Table 3 are derived for a single (mean) position even for the Na atom. Nevertheless, with *mean* high albite distances in place of (monoclinic) sanidine distances, individual Na–O distances in (ordered) low albite show the same type of variation as individual K–O distances in (ordered) microclines.

The features found to be characteristic of the change from Al,Si disorder to a high degree of Al,Si order are thus the same in both potassium and sodium feldspars. Table 3 also shows that reedmergnerite, the boron analogue of low albite, shows the same trends except for the pair of atoms  $O_C(0)$  and  $O_C(m)$ ; this special feature is considered in § 3, in which the K (or Na)–O bond lengths are correlated with the tetrahedral bond lengths in the structures.

### 3. Interpretation of K (Na)–O bond lengths in relation to tetrahedral bonds

The trends in K(Na)–O bond lengths described in § 2 can be correlated with tetrahedral bond lengths in the

Table 1. K–O distances in potassium feldspars (Å)

Distance	Sanidine (a)	Spencer C (b)	St. Gotthard (c)	Spencer U (d)	Pontiskalk (e)	Pellotsalo (f)
K– $O_{A1}$	2.924	2.901	2.907	2.889	2.883	2.879
– $O_{A2}$	2.710	2.697	2.728	2.750	2.743	2.750
– $O_B$	3.037	3.051	3.049	3.040	3.050	3.048
– $O_C$	3.136	3.128	3.129	3.110	3.131	3.121
– $O_D$	2.954	2.937	2.954	2.951	2.941	2.943
Total Al in $T_1$	0.55	0.64	0.64	0.96	0.92	0.97

- Notes (1) In this Table for the triclinic materials the distances to pairs of O atoms of different types (e.g. K– $O_B$ ) are average values; in Table 2 the separate values are quoted.  
 (2) For standard deviations or estimated errors in the values quoted, the original publications should be consulted. For Spencer U a previously undetected arithmetical error has been corrected in calculating the values now quoted, the only significant differences being in the distances K– $O_B$  and K– $O_C$ .  
 (3) The amount of Al in a tetrahedral site  $T_1$  is derived from the measured size of the tetrahedron by use of the Smith & Bailey (1963) relation with total Al adjusted to 1.00.  
 (4) References: (a) Sanidinized Spencer C orthoclase: Cole, Sörum & Kennard (1949), Ribbe (1963), Jones (in preparation) (re-refinement, provisional figures). (b) Jones & Taylor (1961), Jones & Taylor (in preparation) (re-refinement, provisional figures). (c) Jones & Taylor (in preparation) (provisional figures). (d) Bailey & Taylor (1955) (see note (2) above). (e) Finney & Bailey (1964). (f) Brown & Bailey (1964).

Table 2. K–O distances (Å) and T–O linkages in potassium feldspars

Distance	T–O linkages	Sanidine	Spencer U	Pontiskalk	Pellotsalo
K– $O_{A1}(0)$	Al+Si	2.924	2.885 –0.039	2.876 –0.048	2.877 –0.047
– $O_{A1}(c)$	Al+Si	2.924	2.894 –0.030	2.890 –0.034	2.881 –0.043
– $O_{A2}(0)$	Si+Si	2.710	2.750 +0.040	2.743 +0.033	2.750 +0.040
– $O_B(0)$	Al+Si	3.037	2.983 –0.054	2.961 –0.076	2.961 –0.076
– $O_B(m)$	Si+Si	3.037	3.097 +0.060	3.139 +0.102	3.136 +0.099
– $O_C(0)$	Al+Si	3.136	3.011 –0.125	2.923 –0.213	2.907 –0.229
– $O_C(m)$	Si+Si	3.136	3.209 +0.073	3.338 +0.202	3.335 +0.199
– $O_D(0)$	Al+Si	2.954	2.919 –0.035	2.903 –0.051	2.892 –0.062
– $O_D(m)$	Si+Si	2.954	2.984 +0.030	2.979 +0.025	2.993 +0.039
Al in $T_1(0)$		0.27	0.69	0.90	0.94

- Notes (1) For this Table, Notes (2) (3) (4) of Table 1 are relevant.  
 (2) The T–O linkages for the individual O atoms correspond to the perfectly ordered Al, Si distribution.  
 (3) For each triclinic material the length of each K–O contact is shown and also the increase (+) or decrease (–) compared with the length of that contact in sanidine (sanidinized orthoclase).

ordered alkali feldspar structures if linkages O to (Al+Si) and O to (Si+Si) are distinguished, on the assumption that the ionic charge on K or Na is satisfied by contacts with atoms  $O_{A1}(0)$ ,  $O_{A1}(c)$ ,  $O_B(0)$ ,  $O_C(0)$  and  $O_D(0)$ . For each of these atoms – group I in Table 4 – has linkages to Al and Si; each of the atoms  $O_{A1}$  is also bonded to *two* K (or Na) atoms, while each atom  $O_B(0)$ ,  $O_C(0)$ ,  $O_D(0)$  is also bonded to *one* K (or Na) atom. That these O–K (or Na) contacts

are to be regarded as bonds follows from their systematic shortening (Tables 2 and 3) in the ordered structures – whereas contacts with  $O_{A2}$ ,  $O_B(m)$ ,  $O_C(m)$ ,  $O_D(m)$ , (group II in Table 4), longer in the ordered structures, are non-bonding. That there is a real physical difference between the O atoms in group I and those in group II is confirmed by the systematic differences in tetrahedral bond lengths listed in Table 4. Thus O atoms in group I have a bond close to 1.74 Å

Table 3. Na–O distances (Å) in sodium feldspars

Distance	High albite (a)		Low albite (a)	Reedmergnerite (b)
	mean			
Na– $O_{A1}(0)$	2.60		2.66	2.455
– $O_{A1}(c)$	2.71	2.65	2.54	2.489
– $O_{A2}(0)$	2.34	2.34	2.38	2.397
– $O_B(0)$	2.53		2.46	2.410
– $O_B(m)$	3.17	2.85	3.47	3.117
– $O_C(0)$	3.37		2.95	3.452
– $O_C(m)$	2.91	3.14	3.26	2.808
– $O_D(0)$	2.51		2.44	2.380
– $O_D(m)$	3.13	2.82	2.99	2.860

## Notes

- (1) References: (a) Ribbe, Megaw & Taylor (1968). (b) Appleman & Clark, 1965.  
 (2) The physical significance of the Na–O distances is discussed in the text.

Table 4. Tetrahedral bond lengths (Å) in highly ordered alkali feldspars

Structure	O atoms in group I								O atoms in group II			
	Al to				Si to				Si to			
	$O_{A1}$	$O_B(0)$	$O_C(0)$	$O_D(0)$	$O_{A1}$	$O_B(0)$	$O_C(0)$	$O_D(0)$	$O_{A2}$	$O_B(m)$	$O_C(m)$	$O_D(m)$
Pellotsalo	1.738	1.739	1.745	1.741	1.592	1.574	1.593	1.592	1.614	1.608	1.629	1.627
(means)	1.741 (0.001)				1.588 (0.004)				1.644	1.624 (0.004)		
Pontiskalk	1.757	1.719	1.722	1.741	1.588	1.586	1.613	1.598	1.620	1.627	1.615	1.623
(means)	1.735 (0.008)				1.596 (0.005)				1.635	1.623 (0.005)		
Low albite	1.750	1.746	1.738	1.749	1.601	1.592	1.587	1.604	1.629	1.603	1.622	1.615
(means)	1.746 (0.002)				1.596 (0.003)				1.641	1.621 (0.004)		
Reedmergnerite					1.595	1.585	1.606	1.614	1.634	1.602	1.624	1.618
(means)					1.600 (0.005)				1.646	1.623 (0.004)		

## Note

- (1) Each atom  $O_{A1}$ ,  $O_B(0)$ ,  $O_C(0)$ ,  $O_D(0)$  in group I is involved in bonding with K (or Na) as well as with 1 Al and 1 Si; each atom  $O_{A2}$ ,  $O_B(m)$ ,  $O_C(m)$ ,  $O_D(m)$  in group II is bonded to 2 Si and takes no part in bonding with K (or Na).  
 (2) The 'standard deviation' [defined as r.m.s. deviation from mean/(number in group)<sup>1/2</sup>] is quoted in brackets after each mean T–O bond length.

with Al, and a bond close to 1.59 Å with Si, whereas those in group II have bonds to 2 Si, of average length close to 1.62 Å

Fig. 1 illustrates the interrelationship between O–K (or Na) distances on the one hand and O–Al, O–Si bond lengths on the other. Two atoms  $O_{A1}$  and one atom  $O_{A2}$  are omitted (for greater clarity) from the coordination group around the K atom (shaded) in microcline (Pellotsalo); for each O atom the distance O–K (Å) and the linkages to Al and Si atoms are shown. Then, for example,  $O_C(m)$  is shared by tetrahedra  $T_1(m)$  and  $T_2(0)$  both of which contain Si in the fully ordered structure, and the O–Si distances, determined entirely by the two small  $Si^{4+}$  ions, are nearly identical (1.63 Å in Pellotsalo microcline, Table 4) while the (non-bonding) O–K distance is large (3.34 Å, Table 2). By contrast,  $O_C(0)$  is shared by tetrahedra  $T_1(0)$  containing Al and  $T_2(m)$  containing Si and is bonded to K; the O atom moves away from the large  $Al^{3+}$  ion and so nearer to both  $Si^{4+}$  ion (1.59 Å, Table 4) and  $K^+$  ion (2.91 Å, Table 2), both figures for Pellotsalo microcline. Similarly for other O atoms in the coordination group.

Thus, in the ordered alkali feldspars a model based on ionic bonding between K (or Na) and certain of the O atoms which constitute the cavity occupied by the cation is capable of explaining in a completely self-consistent scheme the details of the K (or Na)–O, Al–O and Si–O interatomic distances throughout the structure. ‘Special features’ such as those mentioned in § 1 receive reasonable explanations within the scheme, in terms of geometrical packing requirements. Thus the extremely short distance  $O_{A2}$ –K (or Na) seen in all feldspars does not indicate a strong bond to the cation, as is seen from the T–O bond lengths for this O atom (Table 4) which are comparable to, though slightly larger than, those for other O atoms not participating in K(Na) bonding.\* A comparable ‘anomaly’ in reedmergnerite, already mentioned in § 2, receives a similar explanation; for the long bonding contact Na to  $O_C(0)$  of 3.45 Å and the short non-bonding contact Na to  $O_C(m)$  of 2.81 Å (Table 3) are associated with Si–O bonds to  $O_C(0)$  and  $O_C(m)$  which are strictly comparable to those of the alkali feldspars. For reedmergnerite the steric factors must be expected to produce quite important distortions of the feldspar geometry since the large aluminium atom is here replaced by the small boron atom. Somewhat similar readjustments have recently been noted in tugtupite (Danø, 1966); here the Si–O distance is 1.588 Å when the O atom is also linked to small, doubly-charged Be

but contracts to 1.566 Å when it is linked to the larger but triply-charged Al.

Finally, the apparent contradiction between bond strengths in the ordered alkali feldspars and those in the (ordered) anorthite structure is probably explicable as arising from two major differences between the structures. First, in anorthite  $AlO_4$  and  $SiO_4$  tetrahedra alternate with perfect regularity in all directions throughout the structure, so that every O atom is linked to 1 Al+1 Si; in the ordered alkali feldspars such alternation is relatively infrequent – necessarily, for composition  $AlSi_3$  – and only one half of the O atoms are linked to 1 Al+1 Si, the remainder to 2 Si. Second, in anorthite the cation is doubly charged and small, against the large  $K^+$  ion in the microclines or the  $Na^+$  ion, with marked anisotropy, in albite. It must, apparently, be accepted that the two structural types require separate discussion and cannot be described by one comprehensive bonding scheme; in anorthite the T–O bond length varies with the number of Ca atoms to which the O atom is linked, in the alkali feldspars the dominating influence on the T–O bond length is whether or not the O atom participates in satisfying the cation charge by forming an ionic bond with K (or Na).

#### 4. Further discussion of tetrahedral bond lengths

The accuracy of the interatomic distances listed in Tables 2, 3 and 4 is ample to establish the conclusions set out in § 2 and § 3 about the nature of the bonding systems in the structures. The further discussion of the tetrahedral bond lengths, which follows, leads to a

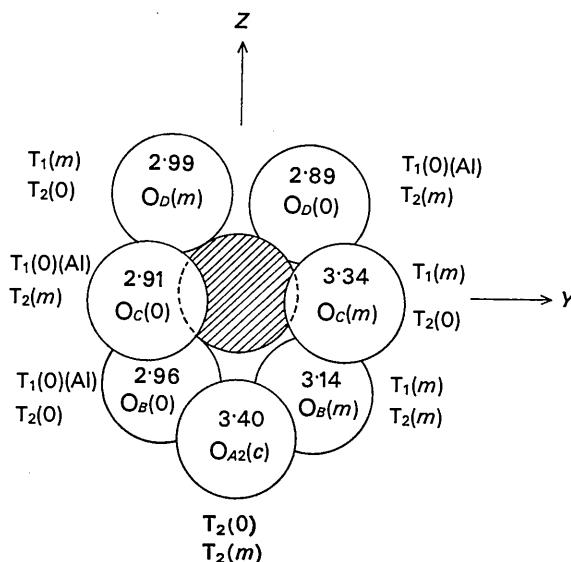


Fig. 1. Coordination group of O atoms around K, in Pellotsalo microcline viewed along  $a^*$ . Two  $O_{A1}$  atoms and one atom  $O_{A2}$  are omitted, for greater clarity. The tetrahedral atoms bonded to each O atom in a fully ordered structure are indicated; atom  $T_1(0)$  is Al, atoms  $T_1(m)$ ,  $T_2(0)$ ,  $T_2(m)$  are Si. (Modified from Brown & Bailey, 1964.)

\* In considering the physical significance of these interatomic distances it is not sufficient to think of the ions as if they were point charges: the electron cloud around  $O_{A2}$  will be displaced towards the adjacent Si ions  $T_2(0)$  and  $T_2(m)$ , and the electron cloud of K will also be distorted from the spherically symmetrical configuration (cf. the discussion of anorthite in Megaw, Kempster & Radoslovich, 1962, page 1031 and Fig. 4).

Table 5. Bond angles at O atoms and T-O distances (Å)

	Pellotsalo microcline			Pontiskalk microcline			Low albite			Reedmergnerite		
	Angle	Si-O	Average T-O	Angle	Si-O	Average T-O	Angle	Si-O	Average T-O	Angle	Si-O	Average T-O
Group I												
T <sub>1</sub> (0)-O <sub>B</sub> (0)-T <sub>2</sub> (0)	151.2°	1.574	1.656	150.9°	1.586	1.653	139.6°	1.592	1.669	140.5°	1.585	1.528
T <sub>1</sub> (0)-O <sub>A1</sub> -T <sub>1</sub> (m)	144.7	1.592	1.665	144.3	1.588	1.673	140.7	1.601	1.676	143.1	1.595	1.537
T <sub>1</sub> (0)-O <sub>D</sub> (0)-T <sub>2</sub> (m)	140.0	1.592	1.667	139.7	1.598	1.670	134.0	1.604	1.677	135.4	1.614	1.541
T <sub>1</sub> (0)-O <sub>C</sub> (0)-T <sub>2</sub> (m)	130.7	1.593	1.669	131.1	1.613	1.668	129.6	1.587	1.663	124.9	1.606	1.525
Group II												
T <sub>1</sub> (m)-O <sub>B</sub> (m)-T <sub>2</sub> (m)	156.0°	1.608	1.612	156.8°	1.627	1.609	161.2°	1.603	1.610	158.1°	1.602	1.611
T <sub>2</sub> (0)-O <sub>D</sub> (m)-T <sub>1</sub> (m)	143.2	1.621	1.624	141.5	1.641	1.632	151.2	1.623	1.619	146.3	1.613	1.616
T <sub>2</sub> (0)-O <sub>A2</sub> -T <sub>2</sub> (m)	138.5	1.614	1.629	138.1	1.620	1.628	130.5	1.629	1.635	128.7	1.634	1.640
T <sub>2</sub> (0)-O <sub>C</sub> (m)-T <sub>1</sub> (m)	130.7	1.633	1.631	131.9	1.629	1.622	135.7	1.641	1.619	135.9	1.646	1.625
		1.629			1.615			1.622			1.625	1.624

Notes

(1) Groups I and II of O atoms as in Table 4.

(2) In each group the O atoms are listed in order of decreasing interbond angle for the microcline structures.

(3) In Group I the average T-O distance is greater than the Si-O distance, the atom T<sub>1</sub>(0) being Al, except in reedmergnerite where T<sub>1</sub>(0) is B.

significant correlation between certain T-O bond lengths and interbond angles at the common O atom.

In Table 4 for each of the highly ordered alkali feldspars the Al-O bond lengths are more nearly constant than the Si-O bond lengths, as is shown by the larger standard deviations for the latter. Table 5 regroups all these bond lengths and also lists T-O-T interbond angles for each O atom, classifying the O atoms into groups I and II as in Table 4.

For O atoms in group II (which do not contribute to K or Na bonding) there is a direct relationship between increase in Si-O-Si interbond angle and decrease in average O-Si bond lengths at that atom; otherwise expressed, the more nearly collinear the two bonds, the shorter their average length and so, presumably, the greater their average strength. Thus a factor external to the particular tetrahedral group under consideration - namely the interbond angle at an O atom - is identified as modifying the tetrahedral bond.

The statistical formulation of the bond angle - bond length relationship is represented by a regression line  $y = 1.7307 - 0.00076x$ , with correlation coefficient -0.88, on plotting average O-Si bond length ( $y$ ) against interbond angle ( $x$ ); the scatter of points is rather large ( $\sigma = 0.004$  to  $0.006$ ), but no point is more distant than twice the standard deviation from the line, and most are within the standard deviation.

For O atoms in group I, which contribute to K or Na bonding, and are linked to 1 Al+1 Si, there is a fair correlation between increase in interbond angle Al-O-Si and decrease in the O-Si bond length, with correlation coefficient -0.6. This is almost identical with the correlation coefficient -0.7 for interbond angle against individual O-Si bond lengths for O atoms in group II, and represents no more than a general trend.

There is no obvious relationship between interbond angle and the average of O-Al and O-Si bond lengths for these same atoms in group I, the correlation coefficient being -0.2.

In considering the relationship thus established between interbond angles and certain T-O bond lengths the possible influence of other factors on bond lengths must not be forgotten - as, for example with O<sub>A2</sub> for which in all structures (Table 4) the bond to Si<sub>2</sub>(m) is significantly longer than the bond to Si<sub>2</sub>(0). Moreover, the demonstration that the relationship holds good does not immediately lead to an explanation of the nature of the forces responsible for it. In this connexion, the observation of a similar relationship in horadaite (Takeuchi & Joswig, 1966) may be of interest.

The measurements which have been analysed in this paper point to the need for caution in any attempt to interpret individual interatomic distances in terms of bond strengths. The particular case of reedmergnerite is perhaps worth emphasizing. Appleman & Clark (1965) in a detailed comparison of the structures of reedmergnerite and albite are led to conclude that since the average Si-O distance in reedmergnerite

is 1.616 Å, significantly greater than the distance associated with a pure Si-O bond in a feldspar by Smith & Bailey (1963), *therefore* the error involved in the use of the Smith & Bailey relation for a feldspar is such that a bond of this length does not necessarily indicate the presence of even a small proportion of Al in the tetrahedral group.

An equally reasonable alternative interpretation is that an O atom in reedmergnerite linked to the triply charged B atom (which is much smaller than triply charged Al in the corresponding location in low albite) is so strongly bonded to this atom that its other tetrahedral bond (to Si) is weaker, and so longer, than the corresponding bond in low albite with the result that the SiO<sub>4</sub> tetrahedron is slightly larger than expected for pure Si occupancy in a feldspar. Each of the O atoms in group I of Table 4 is linked to 1 Si and 1 Al (in feldspars) or 1 B (in reedmergnerite): the mean Si-O distances in this group show a trend in the direction to be expected if this interpretation is valid - thus reedmergnerite 1.600 Å, but low albite and Pontiskalk microcline 1.596 Å, Pellotsalo microcline 1.588 Å. The differences are, however, too small to be statistically significant and no definite conclusion can be reached on the basis of these figures alone.

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