The Structures of Monoclinic Potassium-Rich Feldspars

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Abstract

The crystal structures of a low sanidine and an adularia (a = 8.539(4), 8.545(2); b = 13.015(5), 12.967(5); c = 7.179(3), 7.201(3)Å; β = 115.99(2), 116.00(2)°; $2V_\alpha$ = 22°, 65°; space groups $C2/m$) have been refined to R = 0.043 and 0.046, respectively. The mean T-O distances are $\langle T_1-O \rangle$ = 1.650, 1.665Å; $\langle T_2-O \rangle$ = 1.637, 1.621Å yielding by the linear model of Ribbe and Gibbs (1969) the following average aluminum contents: Al_{T_1} = 0.29(2), 0.40(2); Al_{T_2} = 0.21, 0.11. The low sanidine values agree well with a neutron diffraction site refinement of the same material by Brown *et al.* (1971): Al_{T_1} = 0.32(2); Al_{T_2} = 0.18.

Multiple linear regression analysis of data from these two and three previous structure refinements of monoclinic K-rich feldspar indicates that the parameters influencing individual T-O bond length variations are, in order of importance: aluminum content of the T site, $-1/\cos(T\text{-}O\text{-}T)$, $\Sigma[1/(K\text{-}O)^2]$ and the aluminum content of the bridging T site. Expressing aluminum content of the T_1 and T_2 tetrahedra in terms of the cell-edge parameter ($c - 0.4b$) and assuming average values of $-1/\cos(T\text{-}O\text{-}T)$ and $\Sigma[1/(K\text{-}O)^2]$ for each of the oxygen atoms, eight equations of the form $(T\text{-}O)_i = p_i + q_i(c - 0.4b)$ have been obtained which predict individual bond lengths that are in excellent agreement with those observed.

Introduction

Because of the petrologic importance of the feldspars, much interest has focused on the problem of relating easily measured parameters to structural state (Wright and Stewart, 1968; Stewart and Ribbe, 1969; Hovis, Waldbaum and Thompson, 1970; Ribbe, 1972). Structural state is dependent on the average Al/Si occupancy of the non-equivalent tetrahedra, which is established either from the mean T-O bond lengths (Smith and Bailey, 1963) or from results obtained in a site occupancy refinement (Fischer and Zehme, 1967; Brown *et al.*, 1971). In addition to structural state, interest has recently centered on the nature of bonding in the feldspars as related to the variation of individual T-O bond lengths (Jones and Taylor, 1968; Brown, Gibbs, and Ribbe, 1969; Phillips, Colville, and Ribbe, 1971; Phillips, Ribbe, and Gibbs, 1972).

The data used in our study of bond length variation in monoclinic potassium-rich feldspars are taken from the following sources: Ribbe (1963), sanidine (heated Spencer C); Colville and Ribbe (1968), orthoclase (Spencer C) and adularia (Spencer B). Two new structure analyses are reported for an adularia (#7007) from St. Gotthard, Switzerland, and for a low sanidine (#7002) from Laacher See, Eifel District, Germany. These were obtained from a suite of feldspars studied by Hovis (1971). A structure of low sanidine from the same locality has also been refined by Brown *et al.* (1971) using neutron diffraction. The T-O bond lengths determined by Brown *et al.* are not significantly different from those determined here; thus their data were not included in this study, except for purposes of comparison.

Experimental Procedure

Examination of long-exposure precession photographs of the low sanidine (#7002) and adularia (#7007) revealed that, although intense reflections of the type $h + k = 2n$ appear to be slightly diffuse, there are no observable diffuse reflections of the type $h + k = 2n + 1$ reported in the Spencer B adularia by Colville and Ribbe (1968); accordingly, the space group symmetry of both crystals is assumed to be $C2/m$. The cell parameters were obtained by diffractometer measurements of ϕ and 4θ along the axial zones, and assuming wave lengths of 0.71069 and 0.70926 Å for MoKα and MoKα_1. Cell parameters, electron microprobe analyses and optic axial angles are given in Table 1.

Intensity data were collected for both crystals on an automated four-circle single-crystal diffractometer with a scintillation counter employing Nb-filtered MoKα radiation. The reflections were measured using 2θ scans with 20 second background counts at both the beginning and the end of each scan. A program written by C. T. Prewitt was used to correct the intensity data for background, Lorentz and polarization effects, and to convert the resulting data to $|F_{obs}|$. No absorption corrections were deemed necessary because no dimension of either crystal exceeded 0.12mm.

TABLE 1. Chemical Composition and Cell Parameters

	Adularia (7007)		Low Sanidine (7002)	
	Composition*			
	Wt. percent		Wt. percent	
	cation	oxide	cation	oxide
Si	30.35	64.92	30.29	64.80
Al	9.85	18.61	9.92	18.74
K	12.03	14.49	11.97	14.42
Na	0.96	1.29	1.20	1.62
Fe	0.07	0.09	0.20	0.26
Ca	0.03	0.04	0.01	0.01
TOTAL		99.44		99.85
Mole % albite		11.90		14.60
	Cell parameters**			
a	8.545(2)Å		8.539(4)Å	
b	12.967(5)		13.015(5)	
c	7.201(3)		7.179(3)	
β	116.00(2)°		115.99(2)°	
a^*	0.13021(3)Å^{-1}		0.13029(7)Å^{-1}	
b^*	0.07712(3)		0.07684(3)	
c^*	0.15450(6)		0.15497(7)	
$2V_\alpha$	65(2)°		22(5)°	

* Ba, Sr and Rb were not determined. They have been reported by Hovis (1971) in the KC1-exchanged equivalents of 7002 and 7007.

** Errors are in parentheses and refer to the last decimal place. These errors are arbitrarily taken as twice the estimated standard deviations of the measurements.

There was no evidence of extinction effects. Refinements were carried out on the low sanidine and the adularia using 1114 and 1074 structural amplitudes[1] collected over a $\sin\theta/\lambda$ range of 0.3 to 0.6. Only structural amplitudes of the type $|F_{obs}|$ greater than four times the standard deviation in $|F_{obs}|$ as determined by counting statistics were used in the ORFLS *refinement* (Busing, Martin, and Levy, 1962). In both cases a unitary weighting scheme sufficed to minimize the variation of $\langle w\Delta F^2 \rangle$ over the entire range of $|F_{obs}|$ as suggested by Cruickshank (1965). Atomic scattering factors were taken from Doyle and Turner (1968) assuming neutral atoms. The scattering factors for the tetrahedral atoms and the Na/K atoms were both weighted according to the chemical analyses. The final unweighted

[1] To obtain a listing of the structural amplitudes used in these refinements, order NAPS Document Number 02026 from Microfiche Publications, Division of Microfiche Systems Corporation, 305 East 46th Street, New York, N.Y. 10017. Please remit in advance $1.50 for microfiche or $5.00 for photocopies. Please check the latest issue of this journal for the current address and prices.

TABLE 2. Atomic Coordinates*

Atom	Adularia			Low Sanidine		
	x	y	z	x	y	z
$O_{A(1)}$	0	0.1447(3)	0	0	0.1461(2)	0
$O_{A(2)}$	0.6339(4)	0	0.2848(5)	0.6330(4)	0	0.2851(5)
O_B	.8262(3)	.1449(2)	.2280(4)	.8276(3)	.1453(2)	.2256(4)
O_C	.0339(3)	.3117(2)	.2585(4)	.0330(3)	.3103(2)	.2572(3)
O_D	.1821(3)	.1257(2)	.4070(3)	.1813(3)	.1265(2)	.4038(3)
T_1	.0093(1)	.1842(1)	.2243(1)	.0094(1)	.1843(1)	.2239(1)
T_2	.7078(1)	.1176(1)	.3445(1)	.7079(1)	.1177(1)	.3444(1)
K	.2834(1)	0	.1372(2)	.2839(1)	0	.1366(2)

* Estimated standard errors are in parentheses and refer to the last decimal place.

residuals for the refinements using isotropic and anisotropic temperature factors were 0.063 and 0.043, respectively, for the low sanidine and 0.064 and 0.046 for the adularia. The atomic coordinates (Table 2), T-O bond lengths (Table 3), K-O and O-O distances and O-T-O and T-O-T angles (Table 4) were all taken from the anisotropic refinements. The temperature factors and r.m.s. equivalents are listed in Table 5.

Numerous unsuccessful refinements of Al/Si site occupancy were attempted using the program RFINE (Finger, 1969). However, Brown *et al.* (1971) were able to obtain a site refinement for low sanidine (#7002) with neutron diffraction data. Their analysis gave Al contents of 0.32 and 0.18 Al ($\sigma = 0.02$ Al) for T_1 and T_2, respectively. These are in good agreement with the Al contents predicted from the mean T-O bond lengths obtained in our study.

Discussion

Cole, Sörum and Kennard (1949) pointed out that the average Al content of a tetrahedral site is the most important factor influencing tetrahedral bond length variations in a feldspar. Smith and

TABLE 3. Tetrahedral Bond Lengths (Å)*

T-O	Heated C**	Low Sanidine	Spencer C***	Adularia	Spencer B***
T_1-O_A1	1.643	1.650(1)	1.654(4)	1.663(1)	1.667(2)
-O_B	1.645	1.639(3)	1.641(6)	1.657(3)	1.646(6)
-O_C	1.647	1.657(2)	1.661(7)	1.672(3)	1.670(3)
-O_D	1.643	1.651(2)	1.666(5)	1.669(2)	1.671(4)
Mean T_1-O	1.645	1.650	1.656	1.665	1.664
T_2-O_A2	1.645	1.643(1)	1.641(3)	1.635(2)	1.632(2)
-O_B	1.631	1.632(3)	1.620(6)	1.611(3)	1.623(6)
-O_C	1.638	1.637(2)	1.631(6)	1.620(2)	1.615(5)
-O_D	1.645	1.636(2)	1.621(5)	1.619(2)	1.618(3)
Mean T_2-O	1.640	1.637	1.628	1.621	1.622

* Estimated standard errors are in parentheses and refer to the last decimal place. Errors are not available for heated C.

** Values from Ribbe (1963) T_2-O_C and T_2-O_D distances given here are correct.

*** Values from Colville and Ribbe (1968).

Bailey (1963) and more recently Jones (1968) and Ribbe and Gibbs (1969) have used this fact to determine linear regression equations for predicting Al occupancy of tetrahedral sites from mean T-O bond lengths. These have met with only moderate success, because in addition to Al occupancy there are other factors which exert small but significant influences on the variation of individual tetrahedral bond lengths. For example, Clark and Papike (1967) noted that for ordered alkali feldspars the Si-O bond lengths in Si-O $\rightarrow$ Al linkages are significantly shorter than the Si-O bond lengths in Si-O $\rightarrow$ Si linkages. Jones and Taylor (1968) and Brown, Gibbs, and Ribbe (1969) independently reported an inverse relationship between the inter-tetrahedral angle T-O-T and the included T-O bond lengths. Brown, Gibbs, and Ribbe (1969) and Phillips, Colville, and Ribbe (1971) found that in the case of the plagioclase feldspars, variation of individual T-O distances could also be inversely related to the respective Na/Ca-O distances. In anorthite Megaw, Kempster, and Radoslovich (1962) pointed out that the oxygen atoms involved in longer T-O bond lengths were those with higher coordination numbers. In a recent statistical analysis of the Wainwright and Starkey

TABLE 4. Interatomic Distances (Å) and Angles (Degrees)*

	Adularia (7007)	Low Sanidine (7002)		Adularia (7007)	Low Sanidine (7002)
K/Na-O_A2	2.704(4)	2.690(4)	T_1-O_A1-T_1	144.1(2)	144.9(2)
-O_A1	2.874(2)	2.893(2)	T_2-O_A2-T_2	137.9(2)	137.7(2)
-O_D	2.942(3)	2.938(3)	T_1-O_B-T_2	152.7(2)	152.2(2)
-O_B	3.027(3)	3.013(3)	T_1-O_C-T_2	130.6(2)	130.9(1)
			T_1-O_D-T_2	141.7(2)	141.4(2)
-O_C	3.109(3)	3.123(2)	Mean	141.4°	141.4°

T_1 tetrahedron: O-O distances			T_2 tetrahedron: O-O distances		
O_A1-O_B	2.653(3)	2.623(3)	O_A2-O_B	2.644(4)	2.672(4)
-O_C	2.787(4)	2.756(3)	-O_C	2.566(3)	2.591(3)
-O_D	2.660(2)	2.633(2)	-O_D	2.644(3)	2.666(3)
O_B-O_C	2.774(4)	2.719(3)	O_B-O_C	2.662(3)	2.686(4)
-O_D	2.746(4)	2.726(4)	-O_D	2.672(4)	2.705(3)
O_C-O_D	2.717(4)	2.696(3)	O_C-O_D	2.688(3)	2.711(3)
Mean	2.718	2.692	Mean	2.646	2.672

T_1 tetrahedron: O-T-O angles			T_2 tetrahedron: O-T-O angles		
O_A1-T_1-O_B	106.1(1)	105.8(1)	O_A2-T_2-O_B	109.1(2)	109.4(2)
-O_C	113.4(2)	112.9(1)	-O_C	104.1(1)	104.3(1)
-O_D	105.9(1)	105.8(1)	-O_D	108.7(2)	108.8(1)
O_B- -O_C	111.1(1)	111.2(1)	O_B- -O_C	110.9(1)	110.5(1)
-O_D	111.3(1)	111.9(1)	-O_D	111.6(1)	111.8(1)
O_C- -O_D	108.8(1)	109.2(1)	O_C- -O_D	112.1(1)	111.8(1)
Mean	109.4°	109.5°	Mean	109.4°	109.4°

* Estimated standard errors are in parentheses and refer to the last decimal place.

TABLE 5. Temperature Factors and r.m.s. Displacements*

	Isotropic	Anisotropic (× 10⁴)						r.m.s. displacement (Å)		
Atom	$B(Å^2)$	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	axis 1	axis 2	axis 3
				Adularia (7007)						
O_A1	1.70(6)	81(5)	21(1)	115(7)	0	49(5)	0	0.132(5)	0.147(5)	0.160(4)
O_A2	1.39(5)	65(4)	14(1)	96(6)	0	17(4)	0	.108(5)	.129(5)	.167(5)
O_B	1.92(5)	77(3)	33(1)	125(5)	-5(2)	63(4)	2(2)	.120(4)	.168(4)	.172(3)
O_C	1.41(4)	57(3)	18(1)	95(4)	-6(1)	26(3)	-6(2)	.114(3)	.139(3)	.149(3)
O_D	1.44(4)	69(3)	20(1)	71(4)	1(1)	19(3)	4(2)	.117(3)	.134(3)	.157(3)
T_1	0.87(2)	41(1)	13(1)	50(1)	-3(1)	22(1)	-3(1)	.097(2)	.102(2)	.116(1)
T_2	0.72(2)	33(1)	9(1)	49(1)	0(1)	18(1)	2(1)	.086(2)	.099(2)	.103(1)
K/Na	2.06(2)	65(1)	36(1)	128(2)	0	30(1)	0	.139(1)	.173(7)	.174(6)
				Low Sanidine (7002)						
O_A1	1.53(5)	86(4)	19(1)	88(5)	0	45(4)	0	0.129(9)	0.129(9)	0.160(9)
O_A2	1.36(5)	66(4)	13(1)	98(5)	0	16(4)	0	.104(5)	.129(4)	.170(4)
O_B	1.91(5)	70(3)	33(1)	118(5)	-8(2)	52(3)	1(2)	.124(4)	.159(3)	.173(3)
O_C	1.34(4)	53(3)	17(1)	91(4)	-5(1)	22(3)	-6(1)	.111(3)	.134(3)	.149(3)
O_D	1.46(4)	66(3)	21(1)	76(4)	2(1)	18(3)	2(1)	.121(3)	.137(3)	.156(3)
T_1	0.70(2)	31(1)	11(1)	37(1)	-4(1)	14(1)	-2(1)	.085(2)	.092(2)	.106(1)
T_2	0.63(2)	28(1)	8(1)	40(1)	-1(1)	12(1)	-1(1)	.083(1)	.091(1)	.098(1)
K/Na	2.10(2)	64(1)	36(1)	131(2)	0	29(1)	0	.138(2)	.175(7)	.176(7)

* Estimated standard errors are in parentheses and refer to the last decimal place. These data were obtained using an average scattering factor for both tetrahedral sites.

(1971) anorthite data, Phillips, Ribbe, and Gibbs (1972) found that for both the Al-O and the Si-O bond length populations, two independent parameters, $\Sigma[1/(Ca-O)^2]$ and $-1/\cos(T$-O-$T)$, are sufficient to describe the variation of individual T-O bond lengths. The parameter $\Sigma[1/(Ca-O)^2]$ accounts not only for the variation of Ca-O distance but also for coordination number effects of the oxygen atoms, whereas the parameter $-1/\cos(T$-O-$T)$ was found to be more highly correlated to individual T-O distances than the T-O-T angle itself (see Gibbs *et al.*, 1972; and an analysis of tetrahedral bond length variation in all feldspars by Ribbe, Phillips and Gibbs, 1973).

Applying the information gained in previous studies, we used multiple linear regression techniques to find the parameters related to individual bond lengths in the monoclinic potassium feldspars. The parameters chosen as independent variables are: (1) the Al content of the T sites calculated using the equation of Ribbe and Gibbs (1969) (these values are shown in Figure 1); (2) the angular parameter $-1/\cos(T$-O-$T)$; (3) $\Sigma[1/(K-O)^2]$; and (4) the Al content of the bridging T site involved in the T-O-T linkage.

TABLE 6. Results of the Multiple Regression Analysis on 40 T-O Bond Lengths

Variable	Regression coefficient	Computed t	Partial corr. coef.
Al content	0.132(12)	11.46	0.889
$-1/\cos(T$-O-$T)$	0.046(9)	5.12	0.654
$\Sigma[1/(K-O)^2]$	0.070(19)	3.73	0.533
Al content of bridging T site	-0.036(12)	-3.15	-0.469

Multiple r = 0.95   Intercept = 1.552

In order to obtain values for the variable $\Sigma[1/(K-O)^2]$, it is necessary to choose a coordination number for the potassium atom. This choice is difficult because the K-O distances range from 2.7 Å to 3.1 Å with no well defined break (see Table 4). In the monoclinic feldspars only the potassium and its nearest oxygen neighbor O_A2 lie on the mirror plane; therefore, all K-O distances except K-O_A2 occur as symmetrically related pairs. In order to assign a coordination number to the potassium, three sets of values for the variable $\Sigma[1/(K-O)^2]$ were calculated assuming the potassium coordination to be five, seven and nine, respectively. Each set of $\Sigma[1/(K-O)^2]$ values was tested in a multiple regression in the presence of the other three independent variables. Examination of statistical parameters indicates that the assumptions of 5- and 7-coordinated potassium give equally good fits; however, the 9-coordinated potassium model is significantly poorer. Thus the potassium atom was *arbitrarily* assigned a coordination number of seven which was used in all subsequent calculations.

After $|t|$ tests (see Table 6) indicated that all four independent variables are statistically significant, a stepwise multiple regression analysis was calculated in order to gauge the contribution of each variable to the regression sum of squares. This analysis indicates that of the four independent variables tested, Al content is by far the most important factor influencing variation in T-O distances. This finding was anticipated; however, at first glance the ranking of the remaining variables appears to be at variance with the results of previous studies. In a similar investigation of low structural state sodic plagioclases, linkage was found to rank second in importance (Phillips, Colville and Ribbe, 1971) whereas in anorthite the parameter $\Sigma[1/(Ca-O)^2]$ is second to site occupancy in importance (Phillips, Ribbe, and Gibbs, 1972), yet this study indicates that in mono-
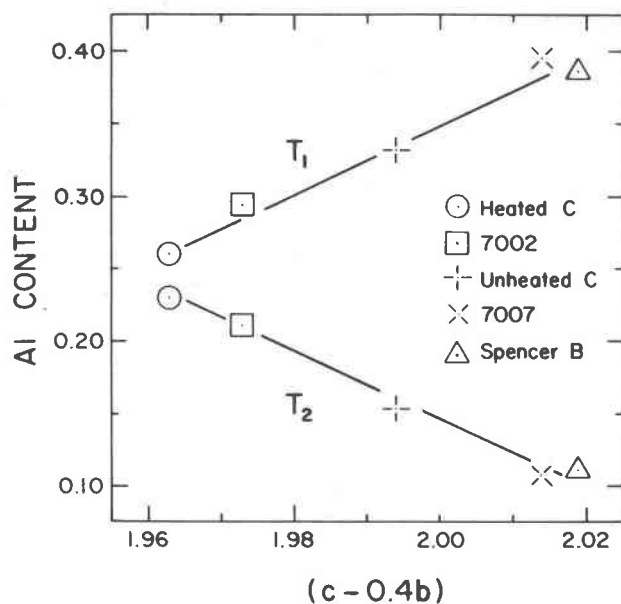

FIG. 1. Plots of the Al contents of T_1 and T_2 calculated using the Ribbe and Gibbs (1969) equation against the structural state parameter ($c - 0.4b$). It is interesting to note that although the two lines are independently determined, their intersection is very near the value 0.25 Al, as would be expected. The correlation coefficients for the T_1 and T_2 data are 0.989(8) and -0.992(6) respectively.

clinic potassium feldspars the second most important parameter is $-1/\cos(T\text{-}O\text{-}T)$ followed by $\Sigma[1/(K\text{-}O)^2]$ and finally by the linkage factor (Al content of the bridging T site). The small effect of the linkage factor is due to the considerable disorder exhibited by the monoclinic feldspars. The small contribution of $\Sigma[1/(K\text{-}O)^2]$ is attributed to the similarity of the potassium-containing polyhedra in all five structures. The largest observed difference in any given K-O distance among these structures is less than 0.04 Å. These variations are relatively small when compared to those in the potassium-containing polyhedra of the triclinic potassium feldspars (Brown and Bailey, 1964; Finney and Bailey, 1964; Bailey, 1969). In light of the much greater variability of the M-O distances (where $M = $ K, Na or Ca) among the triclinic feldspars, it is anticipated that a parameter of the form $\Sigma[1/(M\text{-}O)^2]$ would be more sensitive for triclinic than for monoclinic feldspars.

In summary, the predominant factor influencing individual T-O bond lengths in feldspars is aluminum content of the tetrahedral site. Of less importance are linkage, $-1/\cos(T\text{-}O\text{-}T)$ and $\Sigma[1/(M\text{-}O)^2]$ which accounts for both M-O distance and oxygen coordination number. The linkage factor assumes its greatest role in the ordered alkali feldspars, becoming progressively less important with either increasing disorder or, in the plagioclases, with increasing Ca content. The effect of $\Sigma[1/(M\text{-}O)^2]$ is least in the monoclinic alkali feldspars, where the potassium polyhedra show little variation, and greatest in the Ca-rich plagioclases (in part due to the divalent nature of calcium). The T-O-T angle apparently exerts an appreciable influence on individual T-O bond lengths in all feldspar structures (Ribbe, Phillips, and Gibbs, 1973).

Results

The predicted Al contents of T_1 and T_2 plotted against the structural state parameter $(c - 0.4b)$ (Hovis, Waldbaum, and Thompson, 1970) are shown in Figure 1. The parameter $(c - 0.4b)$ like the parameter (Δbc) (Stewart and Ribbe, 1969) is dependent primarily on Al/Si distribution and is relatively insensitive to sodium content of potassium-rich monoclinic feldspars (Hovis, 1971). A linear least-squares fit of the data presented in Figure 1 yielded the following equations which permit an estimation of the Al content of T_1 and T_2 from the b and c cell edges of monoclinic feldspars:

$$Al_{T_1} = 2.360\,(c - 0.4b) - 4.369;$$
$$\text{corr. coeff.} = 0.989(8) \quad [\text{Eqn. 1}]$$
$$Al_{T_2} = -2.256\,(c - 0.4b) + 4.658;$$
$$\text{corr. coeff.} = -0.992(6) \quad [\text{Eqn. 2}]$$

These equations define, in terms of b and c, two of the four variables (Al content of the T site and Al content of the bridging T site) found to influence the individual T-O bond lengths.

In the previous section it was noted that respective K-O bond distances vary little among the five structures considered. The same is true for respective T-O-T angles, the maximum variation for any given T-O-T angle amongst all five structures being only 1.1 degree. Because the variation of any given K-O distance or T-O-T angle is relatively small, it was decided to calculate an average value for each K-O distance and each T-O-T angle in the monoclinic structure using the data from the five refinements, as listed below:

	$\langle$K-O$\rangle$	$\langle$T-O-T$\rangle$
O_A1	2.890 Å	144.60°
O_A2	2.706	137.92
O_B	3.025	152.64
O_C	—	131.04
O_D	2.945	141.64

Thus the parameters $\Sigma[1/(K\text{-}O)^2]$ and $-1/\cos(T\text{-}O\text{-}T)$ calculated using these values are assumed to be constant for each oxygen in all monoclinic potassium-rich structures. Using these average values of $\Sigma[1/(K\text{-}O)^2]$ and $-1/\cos(T\text{-}O\text{-}T)$ along with the relationships defined by Equations 1 and 2, it is possible to convert the multiple regression equation (Table 6) obtained for all forty T-O distances into eight predictive equations for the eight non-equivalent T-O bond lengths. An example is given in the Appendix. These equations are of the form $(T\text{-}O)_i = p_i + q_i(c - 0.4b)$ where b and c are the cell edges; values p and q for each T-O bond are given in Table 7. Within each tetrahedron the equations for the bond lengths $T\text{-}O_B$, $T\text{-}O_C$ and $T\text{-}O_D$ differ only in the value of the intercept (see Table 7).

Using the equations given in Table 7, the T-O bond lengths were calculated for the five structures, and a plot of these values against the observed distances is shown in Figure 2. A least-squares fit of these data ($\hat{\sigma} = 0.005$Å) yielded a correlation coefficient of 0.959 indicating that the approximations made for $-1/\cos(T\text{-}O\text{-}T)$ and $\Sigma[1/(K\text{-}O)^2]$ are reasonable. The

TABLE 7. Equations for Prediction of Individual T-O Bond Lengths*

Bond length	Intercept	Coefficient
T_1-O_A1	1.205	0.2265
$-O_B$	0.867	0.3927
$-O_C$	0.877	0.3927
$-O_D$	0.874	0.3927
T_2-O_A2	2.071	−0.2166
$-O_B$	2.384	−0.3828
$-O_C$	2.394	−0.3828
$-O_D$	2.391	−0.3828

* Bond length = Intercept + Coefficient × $(c - 0.4b)$

heavy line shown in Figure 2 represents the ideal slope for a perfect correspondence of observed and calculated values; however, the calculated least-squares line which is not shown is very similar, having a slope of 45.4° and an intercept of −0.02Å. Further examination of Figure 2 reveals that the largest differences between observed and calculated distances corresponds

for the most part to bond lengths which have large experimental errors.

These five K-rich feldspars contain 8 to 15 mole percent albite; however, in light of the relative insensitivity of $(c - 0.4b)$ to sodium content and the relatively small contribution of the parameter $\Sigma[1/$ K-O$)^2]$, Na substitution for K should not seriously restrict the applicability of these equations for monoclinic structures.

A test of these equations is illustrated in Figure 3. The solid lines are the equations from Table 7; the dashed lines represent least-squares fits to the five observed T-O distances used in this study. Ideally these two sets of lines should be coincident, and in fact agreement is reasonable except for T_1-O$_B$. In order to check this discrepancy we plotted individual T-O distances from two neutron diffraction refinements of monoclinic K-rich feldspars. The data of Brown *et al.* (1971) are in good agreement with both sets of lines, but the bond lengths of Prince, Donnay and Martin (1972; personal communication from Martin) are in most of the cases better approximated by the equations of Table 7 than the least-squares lines.

FIG. 2. A graph of the observed individual T-O distances of the five structures plotted against the distances predicted using the equations of Table 7. The correlation coefficient for these data is 0.959(5). The horizontal lines represent the errors reported for the observed bond lengths. No experimental errors are available for the high sanidine (heated C) data.
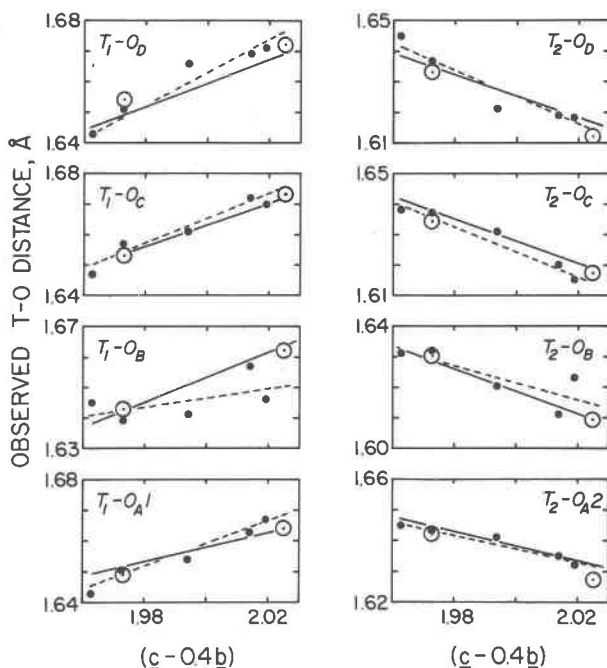

FIG. 3. Plots of the observed bond lengths (small solid circles) used in this study against the parameter $(c - 0.4b)$. The dashed lines represent the least-squares fits for these data whereas the solid lines represent the equations from Table 7. The large open circles represent data from two neutron diffraction refinements which were not used to determine either the dashed or the solid lines.

Acknowledgments

Appendix—Example of Calculation of Equations to Predict Individual T-O Distances

From Table 6 we write the equation:

$$T_1-O_B = 1.552 + 0.132(Al_{T_1})$$
$$+ 0.046(-1/\cos \langle T-O_B-T\rangle)$$
$$+ 0.070(\Sigma 1/\langle K-O_B\rangle^2) - 0.036(Al_{T_2})$$

where $\langle T-O_B-T\rangle$ is the mean $T-O_B-T$ angle and $\langle K-O_B\rangle$ the mean K-O distance listed in the text. Substituting Equations (1) and (2) for Al_{T_1} and Al_{T_2} and evaluating the remaining terms, we obtain $T_1-O_B = 1.552$

$$+ [0.3115(c - 0.4b) - 0.577] + 0.052$$
$$+ 0.008 - [-0.0812(c - 0.4b) + 0.168]$$

which reduces to

$$T_1-O_B = 0.3927(c - 0.4b) + 0.867.$$

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