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The Refinement of the Crystal Structure of a Synthetic Non-Stoichiometric Sr Feldspar

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Abstract

The crystal structure of a synthetic Sr feldspar with vacancies on the alkali cation site has been refined in space group $C2/m$ using 3-D counter diffractometer data and full-matrix least-squares methods. The chemical composition of the feldspar is $Sr_{0.84}Na_{0.03}\square_{0.13}Al_{1.69}Si_{2.29}O_8$ with cell parameters $a = 8.3282(8)$ Å, $b = 12.9801(12)$, $c = 7.1358(6)$, $\beta = 115.599(3)°$. The weights, $1/\sigma^2$, were used throughout the refinement and the final weighted R-factor for 1193 non-equivalent reflections was 4.0 percent. The average Al/Si distribution over the T_1 and T_2 sites determined by least-squares refinement are 0.48(8)Al and 0.39(8)Al, respectively.

Introduction

Recent synthetic work by Grove and Ito (1973) on the ternary system $CaAl_2Si_2O_8$–$NaAlSi_3O_8$–$SrAl_2Si_2O_8$ has shown that the variation in symmetry of the feldspars which occur in this system is a function of both the Al/Si ratio and the alkali cation radius. During the course of this work, spontaneously nucleated single crystals of Sr feldspar were obtained by solvent growth using a V_2O_5 flux. The equilibrated melt was cooled from 1280° to 750°C at a rate of 2°C/hour in a platinum crucible positioned in a silicon carbide muffle furnace so as to be slightly hotter at its bottom; this resulted in a mild stirring of the melt through convection. Single crystals of stoichiometric $Sr_2Al_2Si_2O_8$ were produced from melts with a Al/Si ratio of unity; however, in those melts with Al/Si <1, Sr feldspars were grown with partially vacant alkali cation sites. Subsequent experiments showed that the number of vacancies induced in a particular feldspar was not significantly affected by a change in the Sr concentration of the melt or by the cooling rate.

This paper presents the results of a crystal structure refinement made on one of these non-stoichiometric Sr feldspars of composition corresponding to $Sr_{0.84}Na_{0.03}\square_{0.13}Si_{2.29}Al_{1.69}O_8$ (Table 1). Comments are also made on the role of non-stoichiometry in the formation of myrmekitic intergrowths.

Unit Cell and Space Group

Single-crystal precession photographs displayed diffraction symmetry $C*/*$ consistent with the space groups $C2$, Cm, and $C2/m$. As there is no evidence to suggest the absence of a center of symmetry, the space group $C2/m$ was chosen in accord with other monoclinic feldspars. Long-exposure precession, rotation, and Weissenberg photographs taken with both Cu$K\alpha$ and Mo$K\alpha$ radiation showed that the space group $C2/m$ was not violated by the presence of weak 'b' type reflections as appeared in stoichiometric Sr feldspar which assumes the space group $I2/c$ (Bruno and Gazzoni, 1970). A single crystal which was unzoned, untwinned, and showed sharp optical extinction was selected for the intensity measurements; the unit cell parameters were determined by the least-squares method on 15 reflections collected on a 4-circle diffractometer. All relevant crystal data are presented in Table 1.

Intensity Data

The intensity data were collected on a Syntex P$\bar{1}$ 4-circle diffractometer using monochromatic Mo$K\alpha$ radiation (graphite monochromator and $\lambda = 0.71069$) and the θ-2θ scan method. 1193 intensities were collected out to a 2θ of 65 degrees. Due to the highly absorbing nature of Sr, the data were corrected for absorption using an 8 point gaussian

TABLE 1. Crystal Data

	Wt.%*	Atomic Ratios**				
SiO_2	44.3	Si	2.29		a	8.3282(8) Å
Al_2O_3	27.7	Al	1.69	Tetrahedral ions Σ= 3.99	b	12.9801(12)Å
Fe_2O_3***	0.05	Fe^{3+}	0.00		c	7.1358(6) Å
V_2O_5	0.3	V^{5+}	0.01		β	115.599(3)°
SrO	27.8	Sr	0.84		V	695.7(4) Å
Na_2O	0.30	Na	0.03		Space group	C2/m
CaO	0.03	Ca	0.00	Large cation Σ= 0.87	Z	4
BaO	0.00	Ba	0.00		Linear absorption coefficient	79.60 $cm.^{-1}$
K_2O	0.00	K	0.00		Crystal size	0.14 x 0.10 x 0.08 mm.
	100.45				Radiation	Mo (λ = 0.71069)
					No, of non equivalent reflections $\|F_{obs}\| > 0$	893
					Final R (weight $1/\sigma^2$)	4.0%
					Density (calc)	2.98
					Density (obs)	2.99

*Analysis by Jun Ito **Calculation based on 8 oxygens

***Mainly impurities (probe analysis by D. T. Griffen, personal communication P. H. Ribbe)

quadrature integration for polyhedral crystal shape (program by Coppens from X-RAY72[1]); this was facilitated by the choice of a crystal with well-developed crystal faces. Corrections were also made for the Lorentz and polarization effects and background. The resulting F_{obs} (Table 2) were classed as unobserved if their magnitude fell below four standard deviations derived from counting statistics. This procedure resulted in 893 observed reflections.

Refinement

The final positional parameters and temperature factors for sanidine (SV17T, Weitz, 1972) were used as the initial parameters for the least-squares program RFINE (Finger, 1969a,b) and throughout the refinement weights $1/\sigma^2$ were used where σ was the standard deviation of a reflection based on counting statistics. Atomic scattering factors for neutral atoms were taken from Doyle and Turner (1968) and anomalous dispersion corrections from Cromer (1965). Repeated cycles of full-matrix refinement were made first with isotropic temperature factors and then with anisotropic temperature factors and the extinction parameter as proposed by Zachariasen (1968) and resulted in a weighted R-factor of 4.0 percent (weight $= 1/\sigma^2$) for the observed intensities. At this point, the population of the alkali cation site was set to agree with the chemical analysis and the population of the T_1 site was included as a variable; the refinement was continued with the bulk chemistry of the T_1 and T_2 sites constrained to the Al/Si ratio determined by the chemical analysis.

The structure converged with weighted and unweighted R-factors of 3.9 and 5.0 percent, respectively, for the observed 893 intensities and 4.0 and 7.3 percent for all of the 1193 intensities measured. The weighted R-factors for intervals of magnitude of F_{obs} showed no systematic effects; however, the weighted R-factors for intervals of sin θ/λ showed a slight systematic increase with increasing size of this parameter, probably because of imperfect correction for absorption.

The final positional parameters and equivalent isotropic temperature factors are presented in Table 3. Interatomic distances and angles were computed using the program ERRORS (Finger, 1969, personal communication) in which the associated standard deviations are those derived from the full matrices of

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[1] X-RAY72 X-ray crystallographic system (Stewart *et al*, 1972).

errors both in the atomic positions and the cell parameters. These are listed in Tables 4 and 5 respectively.

Discussion

The structure of the Sr feldspar is very similar to the structures of the monoclinic K feldspars. This can be illustrated most easily by a comparison of the results of a bond strength calculation (Brown and Shannon, 1973) made on representative monoclinic K feldspars (see Table 5 for references). To emphasize the great similarities, bond strengths were normalized by dividing them by the sum of the bond strengths around the cation and expressing them as a percentage (Table 6). A more detailed examination of the table reveals that, in the case of Sr feldspar, the O_A2 anion site deviates somewhat from the general pattern. This is not unexpected because the differing chemistry of the alkali cation site produces a small change in the internal geometry which is reflected in the lattice parameters. Due to the similar ionic sizes of Sr^{2+} and K^+ (Shannon and Prewitt, 1969), the lattice parameters of sanidine (*a* 8.546, *b* 13.037, *c* 7.178, *β* 115.97, Weitz, 1972) and Sr feldspar (Table 1) are comparable. However, in the Sr feldspar, the effective increase in bond strength between O_A1, O_A2 and O_B and Sr leads to a shortening of the *a* and *b* dimensions and a rotation of the tetrahedron causing a decrease in *c* and *β* relative to sanidine. The shortening of the *a* dimension is further enhanced by vacancies on the alkali cation site, to which it appears to be par-

TABLE 2. Structure Factors for Synthetic Sr Feldspar

TABLE 2, Continued

ticularly sensitive, as may be seen by a comparison of the lattice parameters of this feldspar with those of a stoichiometric Sr-feldspar (*a* 8.389; *b* 12.972; *c* 14.262; β 115.43) examined by Nager, Hoffman, and Nissen (1969).

Tetrahedral Cation Sites

The Al content of each of the tetrahedral sites T_1 and T_2 was determined during the least-squares refinement by varying the population of Al on the T_1 site while applying the following constraints:

TABLE 3. Site Population Atomic Coordinates and Temperature Factors*

Site	Population	x	y	z	B**	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
O_A1	1.0	0	.1329(4)	0	1.14(9)	.00739(91)	.00159(32)	.00560(126)	0	.00415(92)	0
O_A2	1.0	.5951(6)	0	.2843(8)	1.11(9)	.00322(85)	.00075(29)	.00966(146)	0	.00017(93)	0
O_B	1.0	.8201(5)	.1298(3)	.2212(6)	1.56(7)	.00732(65)	.00216(26)	.01108(106)	−.00005(33)	.00526(72)	.00112(43)
O_C	1.0	.0193(5)	.3052(3)	.2518(6)	1.44(7)	.00665(68)	.00170(23)	.00999(111)	−.00039(33)	.00350(72)	.00005(40)
O_D	1.0	.1907(5)	.1227(3)	.4025(6)	1.60(7)	.00661(66	.00296(28)	.00660(94)	.00007(35)	.00181(68)	.00069(44)
SI_1	See Table 6	.0054(2)	.1772(1)	.2237(2)	0.74(3)	.00395(23)	.00122(8)	.00339(35)	−.00069(13)	.00196(24)	−.00015(15)
SI_2	See Table 6	.6908(2)	.1166(1)	.3414(2)	0.74(3)	.00387(23)	.00093(9)	.00381(33)	−.00001(11)	.00132(23)	−.00018(14)
SR	0.84Sr + 0.03Na	.2696(1)	0	.1306(2)	2.05(2)	.00610(17)	.00403(9)	.01046(27)	0	.00186(17)	0

*defined as $\exp[-\sum_{i=1}^{3}\sum_{j=1}^{3} h_i k_j \beta_{ij}]$ **$B_{\text{equiv isotropic}}$

TABLE 4. Bond Multiplicities and Interatomic Distances (Å)

T_1 Tetrahedron		
$T_1 - O_A1$	1	1.679(2) Å
$T_1 - O_B$	1	1.653(4)
$T_1 - O_C$	1	1.672(4)
$T_1 - O_D$	1	1.676(5)
Mean $T_1 - O$		1.670

SR Polyhedron		
$SR - O_A1$	2	2.660(4) Å
$SR-- O_A2$	1	2.446(6)
$SR - O_B$	2	2.843(5)
$SR - O_C$	2	3.148(4)
$SR - O_D$	2	2.798(4)
Mean of 7 SR - O		2.721
Mean of 9 SR - O		2.816

T_2 Tetrahedron		
$T_2 - O_A2$	1	1.677(2)
$T_2 - O_B$	1	1.650(4)
$T_2 - O_C$	1	1.640(4)
$T_2 - O_D$	1	1.662(5)
Mean $T_2 - O$		1.657

T_1 Tetrahedron	
$O_A1 - O_B$	2.604(5)
$O_A1 - O_C$	2.830(5)
$O_A1 - O_D$	2.617(7)
$O_B - O_C$	2.769(5)
$O_B - O_D$	2.785(7)
$O_C - O_D$	2.735(5)
Mean O - O	2.723

T_2 Tetrahedron	
$O_A2 - O_B$	2.699(5)
$O_A2 - O_C$	2.592(4)
$O_A2 - O_D$	2.697(7)
$O_B - O_C$	2.740(5)
$O_B - O_D$	2.727(6)
$O_C - O_D$	2.766(8)
Mean O - O	2.704

$$\mathrm{Al}_{T_2} = \mathrm{Al}_{\text{total}} - \mathrm{Al}_{T_1}$$

$$\mathrm{Si}_{T_2} = 1.0 - \mathrm{Al}_{T_2}, \qquad \mathrm{Si}_{T_1} = 1.0 - \mathrm{Al}_{T_1}.$$

The results are given in Table 7. In order to test the validity of these, the Al content of each tetrahedral site was calculated from the mean *T*-O bond length using the equations of Ribbe and Gibbs (1969) and Jones (1968); these are also shown in Table 7, and the agreement is fairly good. A further estimate of the Al content is available from the bond strength calculation made on this feldspar (Table 6); this correlates quite well with the value determined by least-squares refinement. From these results and comparable results on a number of amphiboles (Hawthorne and Grundy, 1973a, b), it is apparent that although the difference between the Al and Si scattering factor curves is extremely small, meaningful estimates may be obtained by this method providing that the major sources of systematic error have been removed from the data. The T_1 site is enriched in Al relative to the T_2 site as is the case in orthoclase.

TABLE 5. Tetrahedral Interatomic Angles (°)

T_1 tetrahedron		T_2 tetrahedron			
$O_A1-T_1-O_B$	102.8(2)°	$O_A2-T_2-O_B$	108.4(2)°	$T_1-O_A1-T_1$	140.0(3)
$O_A1-T_1-O_C$	115.2(2)	$O_A2-T_2-O_C$	102.8(2)	$T_2-O_A2-T_2$	129.0(3)
$O_A1-T_1-O_D$	102.5(2)	$O_A2-T_2-O_D$	107.7(3)	$T_1-O_B-T_2$	148.0(3)
$O_B-T_1-O_C$	112.8(2)	$O_B-T_2-O_C$	112.7(2)	$T_1-O_C-T_2$	131.7(2)
$O_B-T_1-O_D$	113.5(2)	$O_B-T_2-O_D$	110.8(2)	$T_1-O_D-T_2$	140.5(3)
$O_C-T_1-O_D$	109.6(2)	$O_C-T_2-O_D$	113.8(3)		
				Mean T-O-T	138.7
Mean $O-T_1-O$	109.4	Mean $O-T_2-O$	109.4		

TABLE 6. Bond Strength Calculations

	O_A1	O_A2	O_B	O_C	O_D	Σcat
			Sr-feldspar (Sr)[1]			
SR	0.234*	0.371	0.162*	0.093*	0.177*	1.703
T_1	0.862**		0.922	0.878	0.869	3.531
T_2		0.867**	0.929	0.954	0.901	3.650
ΣO	1.958	2.105	2.013	1.925	1.947	
			Adularia (Ad)[2]			
K	0.116**	0.154	0.090*	0.078*	0.102*	0.926
T_1	0.889**		0.939	0.882	0.880	3.590
T_2		0.974**	0.997	1.019	1.011	4.001
ΣO	1.894	2.102	2.026	1.979	1.993	
			Orthoclase (Or)[2]			
K	0.113*	0.156	0.087*	0.076*	0.103*	0.914
T_1	0.920**		0.951	0.903	0.892	3.666
T_2		0.951**	1.005	0.977	1.003	3.940
ΣO	1.953	2.058	2.043	1.956	1.998	
			Sanidine (San)[3]			
K	0.111*	0.163	0.093*	0.074*	0.104*	0.927
T_1	0.939**		0.961	0.951	0.915	3.766
T_2		0.934**	0.959	0.949	0.969	3.811
ΣO	1.989	2.031	2.013	1.974	1.988	

Percentage Charge Contribution of Oxygen to Cations

	O_A1	O_A2	O_B	O_C	O_D
			From Alkali Sites		
Sr	14*	22	10*	6*	10*
Ad	13*	17	10*	8*	11*
Or	12*	17	10*	8*	11*
San	12*	18	10*	8*	11*
			From T_1 Sites		
Sr	24		26	25	25
Ad	25		26	25	25
Or	25		26	25	24
San	24		26	25	24
			From T_2 Sites		
Sr		24	25	26	25
Ad		24	25	25	25
Or		24	26	25	25
San		25	25	25	25

[1] This work. [2] Colville and Ribbe (1968). [3] Weitz, SV17T (1972). *x2 for Σcat. **x2 for ΣO.

The equivalent isotropic temperature factors of the tetrahedral sites (Table 3) are appreciably larger than in anorthite (Wainwright and Starkey, 1971), but comparable with those observed in the monoclinic K feldspars (references, Table 6). This effect can be attributed in part to the Al/Si disorder which exists on both the T_1 and T_2 sites. The anisotropic nature of the vibrational ellipsoids (Table 8, Fig. 1) is probably the result of positional disorder. The

TABLE 7. Occupancies of T_1 and T_2

Reference	T_1		T_1	
	Al	Si	Al	Si
1.	0.42_7	0.57_2	0.34_2	0.65_8
2.	0.42_3	0.57_7	0.34_1	0.65_9
3.	0.46_9	0.53_1	0.35_2	0.64_8
4.	0.48(8)	0.52(8)	0.39(8)	0.61(8)

1. Al/(Al + Si) = 6.58 [<T-O>-1.605] (Ribbe and Gibbs 1969)
2. Al/(Al + Si) = 6.3481 [<T-O>]- 10.178 (Jones 1968)
3. Calculations from bond strength (Brown and Shannon 1973)
4. Occupancies derived by chemically constrained site refinement.

effect of a vacant alkali cation site must cause a relaxation of the surrounding framework; in particular, the tetrahedral cations will be displaced towards the alkali cation site along directions perpendicular to the shared O-O edges. The elongations of the vibrational ellipsoids of the tetrahedral cations were determined from the refined structural parameters and found to lie in the predicted directions (Table 8).

An alternative source of positional disorder would be encountered if the observed $C2/m$ symmetry were in fact an average symmetry. Due to the moderate size of the observed temperature factors, a deviation from $C2/m$ symmetry would not normally be suspected; however, the symmetry of the related stoichiometric Sr feldspar (Bruno and Gazzoni, 1973) and celsian (Newnham and Megaw, 1960) is $I2/c$ as shown by the presence of weak reflections which violate the $C2/m$ symmetry. If the structure of celsian is averaged in the space group $C2/m$, then the resulting positional disorder would produce ellipsoids with elongations on the T_1 and T_2 sites of 0.074 Å and 0.070Å, respectively. These values are close enough to the r.m.s. values for the feldspar under study (Table 8) so as not to preclude the possibility that a disorder of this type contributes to the anisotropy on the tetrahedral sites; the absence of reflections which violate the $C2/m$ symmetry, however, suggests that any deviation from $C2/m$ symmetry must be small and that the high degree of long-range order observed in celsian is not present in this non-stoichiometric feldspar. The presence of short-range order is to be expected because of the clustering of the silica-rich tetrahedra about any vacant alkali cation sites.

TABLE 8. Magnitudes (Å) and Orientation of Thermal Ellipsoids (°)

Atom	r.m.s. displacement	Angle to a-axis	Angle to b-axis	Angle to c-axis
O_A1	0.092(14) Å	120(9)°	90°	5(9)°
	0.116(12)	90	0	90
	0.146(9)	30(9)	90	85(9)
O_A2	0.080(15)	90	0	90
	0.091(13)	142(7)	90	102(7)
	0.166(10)	128(6)	90	12(6)
O_B	0.112(9)	129(12)	129(10)	47(7)
	0.142(7)	140(12)	52(14)	81(14)
	0.163(7)	80(13)	63(13)	45(7)
O_C	0.117(9)	68(14)	22(14)	100(13)
	0.140(7)	147(47)	70(18)	91(64)
	0.146(8)	113(59)	81(26)	10(14)
O_D	0.114(9)	81(10)	102(8)	37(10)
	0.147(7)	161(18)	109(20)	61(13)
	0.163(7)	107(20)	23(18)	69(13)
SI_1	0.077(5)	125(10)	110(14)	24(19)
	0.088(4)	114(12)	132(10)	113(19)
	0.120(3)	45(4)	132(4)	95(4)
SI_2	0.085(4)	91(7)	44(21)	51(17)
	0.093(4)	96(10)	46(21)	126(18)
	0.110(3)	6(10)	85(8)	120(8)
SR	0.128(19)	44(2)	90	71(2)
	0.165(19)	46(2)	90	161(2)
	0.185(18)	90	0	90

Alkali Cation Site

The Sr cation is markedly anisotropic (Table 8, Fig. 1); however, Fourier and difference-Fourier sections through the site reveal no unusual features; its largest vibrations are in directions of least electrostatic resistance, similar to the K feldspars (Brown and Bailey, 1964).

Stoichiometry in the Feldspars

The possibility of non-stoichiometric feldspars has been a much discussed topic since Schwantke (1909) proposed a theory for the origin of myrmekite by the dissociation of the phase $Ca(AlSi_3O_8)_2$ into anorthite and quartz according to the reaction

$$Ca(AlSi_3O_8)_2 \rightarrow CaAl_2Si_2O_8 + 4SiO_2.$$

He argued that such a phase was present in many feldspars which, on chemical analysis, showed an excess of silica.

More recent work on the chemical composition has confirmed that many feldspars do have an excess of silica which cannot be attributed to analytical error (Perry, 1968, p. 211; Sturt, 1970, p. 824; Weill *et al,* 1970; Wenk and Wilde, 1973). Carman and Tuttle (1967) reported on the basis of their experimental work on the alkali feldspar solvus that sanidine can indeed tolerate small amounts of silica in solid solution; in the case of the alkali feldspars this results in an Al/Si ratio less than one-third and

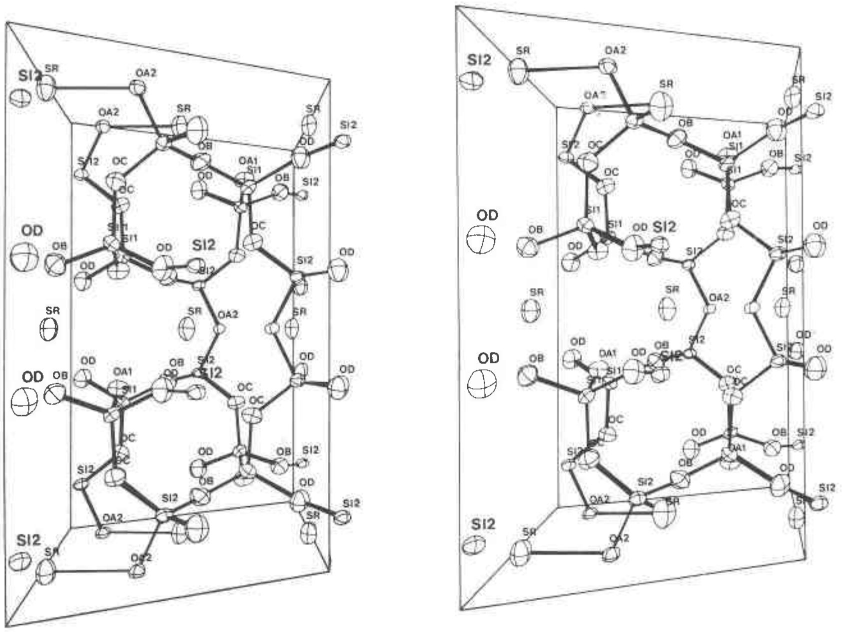

FIG. 1. A stereographic drawing of the Sr-feldspar structure viewed approximately down the direction normal to (001) showing probability ellipsoids of thermal vibration. Solid lines are tetrahedral bond directions associated with the framework; the bonding of Sr to the framework is not shown.

a deficiency of alkali cations. An alternative interpretation of their synthetic data is that the appearance of quartz during the reheating process was due to leaching of the alkalies; however, Morse (1969) discounts this criticism and suggests that the alkali feldspars can indeed be non-stoichiometric.

Preliminary annealing experiments made at 1000°C for two weeks on large crystals of non-stoichiometric Sr feldspar resulted in the appearance of very weak *b*-type reflections on precession photographs exposed for 24 hours (Mo$K\alpha$ radiation). The crystals lost some transparency but no clearly exsolved SiO_2 phase could be detected optically. Similar annealing experiments using a non-stoichiometric synthetic anorthite (J. Ito, in preparation) produced a change in the space group of the anorthite from $C\bar{1}$ to $I\bar{1}$ and finally $P\bar{1}$ and the appearance of a clearly visible exsolved phase, presumably SiO_2. A possible mechanism by which non-stoichiometric Sr and Ca feldspar could exsolve SiO_2 may involve the onset of long range order and thereby generation of stoichiometric Sr and Ca feldspars; the vacant cation sites with the expected short-range ordering of the silica-rich tetrahedra about them would act as nucleation centers for the myrmekitic type intergrowths.

This work provides crystallographic evidence for the existence of a non-stoichiometric feldspar. Although this particular feldspar is not representative of naturally-occurring feldspar compositions and has been grown under somewhat specialized conditions, it seems highly probable that naturally occurring feldspars with a partially-vacant alkali cation site can and do exist, and serious consideration should be given to the effect of these on the physical and chemical properties of feldspar.

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