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Al,Si distribution in a ternary (Ba,K,Na)-feldspar as determined by crystal structure refinement

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Abstract

Refinement of the crystal structure of a ternary barium feldspar with the formula $(Ba_{0.40}K_{0.47}Na_{0.13})(Si_{2.59}Al_{1.41})O_8$, a = 8.544(2), b = 13.030(2), c = 7.195(2)Å, β = 115.68(2)°, space group = $C2/m$ yields a disordered Al,Si distribution, with 0.437 Al in the T_1 site and 0.268 Al in the T_2 site. On the other hand, the lattice parameter c suggests that the investigated specimen probably has a structural state very close to that of maximum order possible for its composition. It is therefore concluded that the state of maximum order for a natural (Ba,K)-feldspar with a Cn (celsian) content of 40 mol% corresponds to a disordered Al/Si distribution. Comparison with the structural data of a Ba-poor feldspar indicates that the disorder shown by such maximum ordered (Ba,K)-feldspars increases with their Cn content.

Introduction

Viswanathan and Kielhorn (1983) have observed that the variations in lattice constants of barium feldspars are similar to those of plagioclases. They concluded that a natural (Ba,K,Na)-feldspar with maximum possible order (as defined by Viswanathan and Brandt, 1980) should exhibit a more disordered distribution with increasing Cn[1] content. In order to prove this statement, Al,Si distributions in natural specimens with different Cn contents are required. The structure of a specimen with the formula $(Ba_{0.19}K_{0.59}Na_{0.22})(Si_{2.82}Al_{1.13}Fe_{0.05})O_8$ has already been reported (Viswanathan and Brandt, 1980). A specimen from Yugoslavia with the chemical formula $(Ba_{0.40}K_{0.47}Na_{0.13})(Si_{2.59}Al_{1.41})O_8$ was chosen for this study.

Experimental and results

The chemical composition was determined by electron microprobe. The crystals were found to be homogeneous and not to contain any unmixed albite or celsian. No attempt was made to determine trace elements such as Sr, Rb *etc*.

The lattice constants determined from a Guinier powder pattern are as follows: a = 8.544(2), b = 13.030(2), c = 7.195(2)Å, and β = 115.68(2)°. The space group is $C2/m$ as determined from precession and Weissenberg photographs. No b-split reflections were observed even after 72 hours of exposure.

The crystal chosen for the structure refinement had an approximate size of 0.06 × 0.18 × 0.4 mm. The calculated linear absorption coefficient, μ, is 32.01 cm^{-1}. The procedure adopted to collect and process the data is the same as that described earlier (Viswanathan and Brandt; 1980). Altogether 1367 reflections were used for the final refinement including the unobserved ones (Table 1)[2], and the final residuals, using isotropic and anisotropic temperature factors, were 0.069 and 0.049, respectively. The atomic coordinates (Table 2) and the important bond lengths and angles (Table 3) were taken from the anisotropic refinement. The temperature factor and the r.m.s. equivalents are listed in Table 4.

Discussion

The relevant structural data of the Cn-poor feldspar (Viswanathan and Brandt, 1980) are included in Tables 2, 3 and 4 for comparison. The atomic coordinates of both are almost identical. The mean

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[1] Cn refers to $BaAl_2Si_2O_8$, celsian.

[2] To receive a copy of the observed and calculated structure factors (Table 1), order Document AM-83-214 from the Business Office, Mineralogical Society of America, 2000 Florida Avenue, N.W., Washington, D. C. 20009. Please remit $1.00 in advance for the microfiche.

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Table 2. Fractional atomic coordinates of Cn-rich and Cn-poor feldspars

Atom	Barium feldspar (Cn-rich)			Barium feldspar (Cn-poor) (Viswanathan and Brandt, 1980)		
	x	y	z	x	y	z
$O_A(1)$	0	.1428(3)	0	0	.1429(2)	0
$O_A(2)$	.6264(5)[a]	0	.2867(6)	.6273(4)	0	.2864(4)
O_B	.8273(4)	.1415(3)	.2274(5)	.8260(3)	.1422(2)	.2270(3)
O_C	.0303(4)	.3104(2)	.2558(4)	.0308)3)	.3101(2)	.2567(3)
O_D	.1842(4)	.1261(2)	.4030(4)	.1841(3)	.1254(2)	.4045(3)
T_1	.0089(1)	.1835(1)	.2242(1)	.0087(1)	.1831(1)	.2240(1)
T_2	.7050(1)	.1179(1)	.3454(1)	.7046(1)	.1175(1)	.3445(1)
(Ba,K,Na)	.2828(1)	0	.1331(1)	.2826(1)	0	.1345(1)

[a] Standard errors $\times 10^{-4}$ are in parantheses.

T–O value (1.655Å) of the specimen under study is larger, which is in accordance with its higher Al-content. The Cn-rich feldspar also shows the characteristic features of the feldspar structure, namely, the smaller $O_A(1)$–T_1–O_B, $O_A(1)$–T_1–O_D and $O_A(2)$–T_2–O_C–angles, and the smaller M–$O_A(2)$-bond (Table 3). The average M–O bonds in both barium feldspars are equal because the higher Ba content and the lower Na content must be compensating in their effects on the M–O bonds of a K-rich ternary feldspar.

The average Al content (Table 5) of the T_1- and T_2-tetrahedra was calculated on the basis of differences in the T–O bond lengths using the method of Ribbe (1975, p. 22). A comparison of the normalized Al,Si distributions shows that the investigated specimen has a more disordered Al,Si distribution than the Cn-poor specimen. An attempt was made to

Table 3. Interatomic distances (Å) and angles (degrees)

	Barium feldspar (Cn-rich)	Barium feldspar** (Cn-poor)		Barium feldspar (Cn-rich)	Barium feldspar (Cn-poor)
T_1-$O_A(1)$	1.669(1)+	1.668(1)	$O_A(1)$-O_B	2.635(2)	2.644(2)
-O_B	1.655(2)	1.653(2)	$O_A(1)$-O_C	2.795(4)	2.795(3)
-O_C	1.668(2)	1.670(2)	$O_A(1)$-O_D	2.641(2)	2.649(2)
-O_D	1.670(2)	1.670(2)	O_B-O_C	2.754(3)	2.747(3)
Mean T_1-O	1.666	1.665	O_B-O_D	2.756(3)	2.752(2)
			O_C-O_D	2.723(3)	2.722(4)
T_2-$O_A(2)$	1.657(1)	1.646(2)	Mean O-O tetrahedron 1	2.717	2.718
-O_B	1.636(2)	1.629(2)			
-O_C	1.638(2)	1.631(2)			
-O_D	1.643(2)	1.637(2)	$O_A(2)$-O_B	2.676(3)	2.666(3)
Mean T_2-O	1.644	1.636	$O_A(2)$-O_C	2.582(2)	2.584(3)
M*-$O_A(1)$	2.865(2)	2.856(2)	$O_A(2)$-O_D	2.678(4)	2.661(3)
-$O_A(2)$	2.651(2)	2.647(2)	O_B-O_C	2.707(3)	2.687(2)
-O_B	2.982(3)	2.995(2)	O_B-O_D	2.712(3)	2.702(3)
-O_C	3.120(2)	3.119(2)	O_C-O_D	2.734(2)	2.715(3)
-O_D	2.932(2)	2.930(2)			
Mean M-O	2.939	2.939	Mean O-O tetrahedron 2	2.682	2.669

T-O-T angles	Ba-Fs Cn-rich	Ba-Fs Cn-poor	O-T-O angles	Ba-Fs Cn-rich	Ba-Fs Cn-poor	O-T-O angles	Ba-Fs Cn-rich	Ba-Fs Cn-poor
T_1-$O_A(1)$-T_1	142.9(3)	143.4(3)	$O_A(1)$-T_1-O_B	104.9(1)	105.5(1)	$O_A(2)$-T_2-O_B	108.7(2)	109.0(1)
T_2-$O_A(2)$-T_2	136.1(2)	136.8(2)	$O_A(1)$ O_C	113.8(2)	113.7(1)	$O_A(2)$ O_C	103.2(1)	104.2(1)
T_1-O_B-T_2	152.0(2)	152.2(1)	$O_A(1)$ O_D	104.6(1)	105.0(1)	$O_A(2)$ O_D	108.5(2)	108.3(1)
T_2-O_C-T_2	130.3(2)	130.9(1)	O_B O_C	112.0(2)	111.5(1)	O_B O_C	111.5(2)	111.0(1)
T_1-O_D-T_2	140.7(2)	141.0(2)	O_B O_D	112.0(2)	111.8(1)	O_B O_D	111.6(1)	111.7(1)
			O_C O_D	109.3(1)	109.2(1)	O_C O_D	112.9(1)	112.4(1)
Mean T-O-T	140.4	140.9						
			Mean	109.4	109.5		109.4	109.4

+ Estimated standard errors are in brackets and refer to the last decimal place.
* M = (Ba,K,Na).
**Viswanathan and Brandt (1980).

Table 4. Temperature factors and r.m.s. displacements

Atom	Isotropic B(Å^2)	r.m.s. displacement (Å)			Anisotropic (x 10^4)					
				Barium feldspar (Cn-rich)						
$O_A(1)$	1.22(7)	0.093	0.121	0.154	78(6)	17(2)	64(7)	0	48(6)	0
$O_A(2)$	1.26(7)	0.151	0.085	0.130	61(6)	8(2)	88(9)	0	22(6)	0
O_B	1.51(5)	0.100	0.161	0.147	69(5)	26(2)	91(6)	-7(2)	53(5)	2(2)
O_C	1.32(5)	0.124	0.109	0.146	64(4)	15(1)	88(6)	-5(2)	41(4)	-4(2)
O_D	1.33(5)	0.145	0.135	0.097	64(4)	21(2)	45(5)	1(2)	18(4)	3(2)
T_1	0.65(2)	0.059	0.090	0.114	39(1)	11(0)	29(2)	-4(1)	24(1)	-2(1)
T_2	0.63(1)	0.077	0.080	0.104	35(1)	8(0)	36(2)	-1(0)	21(1)	0(1)
(Ba,K,Na)	1.42(1)	0.135	0.144	0.119	48(1)	24(0)	84(1)	0	27(1)	0
				Barium feldspar (Cn-poor)*						
$O_A(1)$	1.80(6)	0.131	0.139	0.178	107(5)	23(2)	96(6)	0	55(5)	0
$O_A(2)$	1.80(6)	0.181	0.116	0.149	93(5)	16(1)	109(6)	0	29(5)	0
O_B	2.08(5)	0.131	0.183	0.169	89(3)	37(1)	120(5)	-6(2)	64(3)	0(2)
O_C	1.71(5)	0.148	0.132	0.159	81(3)	22(1)	100(4)	-5(2)	38(3)	-5(2)
O_D	1.70(5)	0.169	0.145	0.122	85(3)	24(1)	72(4)	-3(2)	23(3)	4(2)
T_1	0.95(2)	0.086	0.104	0.133	55(1)	14(0)	41(1)	-5(1)	27(1)	-3(0)
T_2	0.95(2)	0.105	0.099	0.125	52(1)	12(0)	52(1)	0(0)	24(1)	1(1)
(Ba,K,Na)	1.94(2)	0.162	0.167	0.141	67(1)	33(1)	114(1)	0	31(1)	0

Estimated standard errors age given in parantheses and refer to the last decimal place.
*Viswanathan and Brandt (1980).

determine their relative structural states by plotting them or the corresponding ion-exchanged products in Figures 7 and 8 of Viswanathan and Kielhorn (1983). As Figure 7 can be used to estimate the structural states of (Ba,K)-feldspars with Cn content only up to 30% we can conclude that the Cn-poor specimen has not reached the state of maximum possible order because it plots away from a reference-line joining microcline and a (Ba,K)-feldspar with about 35% Cn. This is in agreement with its disordered Al,Si distribution, which is similar to that of Spencer "C". Again, assuming that a line joining microcline and the unmixed Ba-poor specimen in Figure 8 (Viswanathan and Brandt, 1980) represents the boundary line for (Ba,K)-feldspars with maximum possible order, we can conclude that the Cn-rich specimen has a structural state nearer to that of maximum possible order than the Cn-poor variety because the former plots nearer to the boundary line after the ionic exchange. Thus, the Cn-rich specimen, which possesses a structural state nearer to that of maximum possible order, shows a more disordered Al,Si distribution than the natural Cn-poor specimen, though the latter has not reached the state of maximum possible order.

Table 5. Al,Si distributions in barium feldspars and sanidine

Specimen	t_1	t_2	Al in T-sites
Spencer"B"	0.30	0.11	1.0*
Spencer "C"	0.35	0.15	1.0*
Cn-poor feldspar	0.405	0.185	1.18
Cn-rich feldspar	0.437	0.268	1.41
Cn-poor feldspar	0.343	0.156	1.00**
Cn-rich feldspar	0.310	0.190	1.00**

* Data from Colville and Ribbe (1968).
**Total Al normalized to 1.0. See Viswanathan and Brandt (1980).

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