Refinement of the crystal structure of a synthetic non-stoichiometric Rb-feldspar

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ABSTRACT

The crystal structure of hydrothermally synthesized Rb-feldspar (monoclinic, space group C2/m, a = 8.839(2) Å, b = 13.035(2) Å, c = 7.175(2) Å, $\beta = 116.11(1)^\circ$, V = 742.3(3) Å³, Z = 4) has been refined to a final *R* of 0.0574 for 692 independent X-ray reflections. Microprobe analyses of the Rb-feldspar suggest deviation from stoichiometry, with excess Si and Al, resulting in a unit formula of Rb_{0.811} $\Box_{0.127}$ Al_{1.059}Si_{3.003}O₈. Infrared (IR) spectra indicate the structural occupancy of large H₂O content, which implies that the \Box Si₄O₈ substitution favours the structural incorporation of the H₂O molecule at the *M*-site. The mean *T*–O distances are 1.632 Å for *T*1 and 1.645 Å for *T*2, revealing highly disordered (Al,Si) distribution with Al/Si = 0.245/0.755 (*T*1 site) and 0.255/0.745 (*T*2 site).

There are two geochemical implications from this refinement: (1) identification of both rubicline triclinic with (Al,Si) ordered distribution and synthetic monoclinic RbAlSi₃O₈ with (Al,Si) disordered distribution implies that Rb cannot be one of factors disrupting the (Al,Si) ordered and disordered distributions in feldspars; and (2) natural and synthetic feldspars capable of accommodating the large cations tend to incorporate \Box Si₄O₈, excess Al and H₂O components in their crystal structures.

Keywords: Rb-feldspar, \Box Si₄O₈, Al-excess substitution, H₂O molecule.

Introduction

RUBICLINE, the Rb analogue of microcline, (Rb,K)AlSi₃O₈, ideally RbAlSi₃O₈, occurs in several kinds of granitic pegmatites (Teertstra *et al.*, 1997, 1998*b*, 1999*a*). The chemical analyses by electron microprobe show that the 'excess-Si' \Box Si₄O₈ component is normally incorporated into rubiclines, where the maximum limit of solubility is ~5 mol.% \Box Si₄O₈ (Teertstra *et al.*, 1998*a*). However, pure RbAlSi₃O₈ feldspar has never been discovered in nature (e.g. 91 mol.% in Teertstra *et al.*, 1997; 73 mol.% in Teertstra *et al.*, 1998*b*, etc.), and it is not known whether the chemical compositions of Rb-feldspars previously synthesized (e.g. Gasperin, 1971; Voncken *et al.*, 1993) have a stoichiometric RbAlSi₃O₈ composition.

Synthetic Rb-feldspars were grouped topologically into two kinds: (1) the monoclinic structures with space group C2/m comparable to sanidine (Barrer and McCallum, 1953; Ghélis and Gasperin, 1970; Gasperin, 1971; Pentinghaus and Bambauer, 1971; Bruno and Pentinghaus, 1974; Voncken et al., 1993; Koval'skii et al., 2000); and (2) the triclinic structure with space group $C\overline{1}$ analogues to low-microcline (Wietze and Wiswanathan, 1971; Grove and Ito, 1973; McMillan et al., 1980). The crystal structure of monoclinic synthetic RbAlSi₃O₈ feldspar was refined to R = 0.07 using only the isotopic temperature factor (Gasperin, 1971), but the chemical composition was not checked. Therefore, one of the major problems in Rb-feldspar concerns the relationship between the variation in space group due to (Al,Si) ordering and the solubility of the 'excess-Si' \Box Si₄O₈ substitution.

In the present work, we report the refinement of a crystal structure of synthetic non-stoichiometric Rb-feldspar, and discuss the relationship between the structure and deviation from stoichiometry.

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Experimental

Synthesis

Crystals of Rb-feldspar were prepared hydrothermally using the isothermal temperature method. The precursor, a powdered natural albite ($Ab_{98.8}An_{1.0}$) from Minas Gerais, Brazil, was placed in a solvent of RbCl, of which the weight ratio to starting mineral was 20:1. The resulting mixture was inserted into a silver tube containing H₂O up to a filling level of approximately 50%. This tube was sealed and then placed in an autoclave, held at 400°C and an external pressure of 60 MPa. The largest crystals obtained, ~0.1–0.3 mm long, were produced after a run duration of 7 d. The product was a single phase



FIG. 1. SEM photograph of a synthetic Rb-feldspar.



FIG. 2. IR spectrum of synthetic Rb-feldspar.

and of high optical quality, albeit often twinned. The crystals were short prismatic and multifaceted with numerous small pores on the surface (Fig. 1).

Infrared technique

Prior to conducting IR spectroscopy, the samples were heated in an oven at 110° C for 12 h to eliminate H₂O absorbed from atmospheric humidity. Single-crystal IR spectra were obtained using micro-FTIR spectroscopy (Janssen MFT-2000, JASCO) over the range 4000–2500 cm⁻¹ (Fig. 2). Averaged scans were 300 at a nominal resolution of 4 cm⁻¹. The sample was put on the KBr plate with a thickness of 100 µm. The instrument was equipped with a Ge-coated KBr beamsplitter and an MCT detector. The spot size of the beam was ~50 × 50 µm. Measurements were made in air at room temperature.

Chemical analysis

The compositions of the crystals obtained were determined by electron microprobe techniques (JEOL superprobe JXA-8621) at the Chemical Analysis Center, University of Tsukuba, using wavelength dispersion spectroscopy (WDS). The analytical conditions were constrained at a 20 kV accelerating voltage and a 10 nA beam current, using a beam size of 10 μ m. Major elements (Rb, Na, Al, Si) were measured using the synthetic Rb₂ZnSi₅O₁₂ glass (Rb-L α ₁) (Kohn *et al.*, 1994),

with albite (Na- $K\alpha_1$), corundum (Al- $K\alpha_1$) and quartz (Si- $K\alpha_1$) as standards. The elements K, Ca, Sr, Cs, Ba, Pb, Mn, Mg, Fe, Ga, Ti, Ni, P and F were sought, but not detected. Ten analyses obtained along a line from one edge of the crystal to the other are given in Table 1.

X-ray data

The selected crystal exhibited sharp extinction and did not show twinning. Data were collected at the Chemical Analysis Center, University of Tsukuba. The crystal was mounted on an Enraf-Nonius CAD-4 diffractometer, using graphitemonochromatized Mo- $K\alpha$ X-radiation and frame widths of 0.3° in ω , with 60 s spent counting per frame. More than a hemisphere of three-dimensional data was collected within the range of $2^{\circ} \leq 2\theta \leq 70^{\circ}$ in ~72 h. The final unit-cell dimensions were refined on the basis of 25 reflections below $20^{\circ}2\theta$ using least-squares techniques. Comparison between the intensities of equivalent reflections during the data collection showed no evidence of significant decay. The three-dimensional data were integrated and corrected for Lorentz, polarization and background effects using the SDP program (Enraf-Nonius, 1983). An empirical absorption-correction was applied using the ψ -scan technique. A total of 1787 reflections was collected; merging of equivalent reflections gave 1685 unique reflections with 648 classed as observed ($|F_{o}| \ge 4\sigma_{\rm F}$).

| · · · · · · · · · · · · · · · · · · · | | | | | | | | | | | | |
|---------------------------------------|---|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | Aver | age |
| SiO ₂ | 57.67 | 59.40 | 55.12 | 56.93 | 55.22 | 58.92 | 54.69 | 56.75 | 58.03 | 53.87 | 56.66 | (1.58) |
| Al_2O_3 | 17.42 | 17.00 | 16.73 | 17.54 | 17.24 | 18.13 | 15.78 | 16.67 | 16.96 | 16.03 | 16.95 | (0.21) |
| Rb ₂ O | 23.82 | 23.42 | 23.73 | 25.32 | 22.95 | 23.47 | 23.93 | 24.10 | 24.03 | 22.93 | 23.77 | (0.20) |
| Sum wt.% | 98.91 | 99.82 | 95.58 | 99.79 | 95.41 | 100.52 | 94.40 | 97.52 | 99.02 | 92.83 | 97.38 | (3.16) |
| Atomic con | Atomic compositions (a.p.f.u.) normalized to 8 oxygen atoms | | | | | | | | | | | |
| Si | 3.000 | 3.039 | 2.992 | 2.976 | 2.979 | 2.994 | 3.018 | 3.012 | 3.019 | 3.004 | 3.003 | (0.001) |
| Al | 1.068 | 1.025 | 1.069 | 1.081 | 1.096 | 1.086 | 1.026 | 1.043 | 1.040 | 1.054 | 1.059 | (0.001) |
| Rb | 0.797 | 0.770 | 0.827 | 0.851 | 0.796 | 0.767 | 0.849 | 0.822 | 0.807 | 0.822 | 0.811 | (0.001) |
| sum | 4.865 | 4.834 | 4.888 | 4.908 | 4.871 | 4.847 | 4.893 | 4.877 | 4.866 | 4.880 | 4.873 | (0.001) |
| Si+Al | 4.068 | 4.064 | 4.061 | 4.057 | 4.075 | 4.080 | 4.044 | 4.055 | 4.059 | 4.058 | 4.062 | (0.000) |
| Σ charges | 16.001 | 16.001 | 16.002 | 15.998 | 16.000 | 16.001 | 15.999 | 15.999 | 16.003 | 16.000 | 16.000 | (0.000) |
| Si/Al | 2.809 | 2.965 | 2.799 | 2.753 | 2.718 | 2.757 | 2.942 | 2.888 | 2.903 | 2.850 | 2.838 | (0.003) |

TABLE 1. Representative compositions of Rb-feldspar.

Structure solution and refinement

FTIR spectra

The IR spectrum of the chosen crystal is plotted in Fig. 2. A clear absorption peak near 3450 cm^{-1} is due not to humidity absorbed by the sample, but to O–H stretching of structural H₂O molecules (Wilkinson and Sabine, 1973). The spectra are in good agreement with that of sanidine containing H₂O molecules in wavenumber as well as in relative intensities (Beran, 1986). Since the relative intensities of these bands reflect the difference in H₂O content (Ballirano *et al.*, 1996), the strong intensities of absorption bands may indicate a high H₂O content.

Chemistry

In spite of the careful qualitative analyses, Na was not detected in the present crystals. The WDS measurements made at ten different positions on a single crystal sample averaged 56.66 SiO₂, 16.95 Al₂O₃, 23.77 Rb₂O, sum 97.38 wt.% (Table 1), in reasonable agreement with the ideal values of 55.51, 15.70 and 28.79 wt.%, sum 100.00 wt.%. Calculation on the basis of eight oxygen atoms per formula unit (a.p.f.u.) shows that individual values of Rb cations are certainly <1.000 a.p.f.u., while sums of the T-cations are obviously >4.000 a.p.f.u. (Table 1). But Si/Al ratios lower than the ideal (=3.000) corresponding to low Rb cation sums, lying along the same trend for Rbfeldspar (e.g. Teertstra et al., 1999a), lead to adjustment of the total cation charge (=16.000)These deviations from stoichiometry of RbAlSi₃O₈ suggest the possibility of nonstoichiometry for this Rb-feldspar. The high T-cations and low M-cations contents are thought to conform to the KAlSi₃O₈-RbAlSi₃O₈ join (Teertstra et al., 1997, 1998a,b, 1999a,b). The number of T-cations must be constrained to 4.000 a.p.f.u. because of unrecognizable defects in T-cations for the general feldspar formula (Smith and Brown, 1988). Therefore, one of the end-members in the feldspar solid solution corresponds to a $\Box Si_4O_8$ component explaining the "excess of silica" (Grundy and Ito, 1974). Furthermore, excess Al cations are observed for all Rb-feldspars in nature (Teertstra et al., 1998*a*,*b*, 1999*a*). However, the refined crystal resists quantitative analysis of its H₂O content because of its irregular morphology (Fig. 1), although the solubility of hydrogen feldspar HAlSi₃O₈ (Paulus and Müller, 1988) in our IR

| TABLE 2. | Crystallog | aphic param | eters for | Rb-feldspar. |
|----------|------------|-------------|-----------|--------------|
|----------|------------|-------------|-----------|--------------|

| Empirical formula | $Rb_{0.811}\square_{0.127}Al_{1.059}Si_{3.003}O_8$ |
|--|--|
| Formula weight | 386.03 |
| λ (Å) | 0.71073 |
| Crystal system | monoclinic |
| Space group | C2/m |
| a(Å) | 8.839(2) |
| $b(\mathbf{A})$ | 13.035(2) |
| $c(\dot{A})$ | 7.175(2) |
| β(°) | 116.11(1) |
| $V(Å^3)$ | 742.3(3) |
| Z | 4 |
| <i>F</i> (000) | 599.3 |
| D_{cale} (g/cm ³) | 2.776 |
| $\mu (\text{mm}^{-1})$ | 6.06 |
| Crystal size (mm) | $0.12 \times 0.07 \times 0.07$ |
| Max θ (°) | 25 |
| h. k. l ranges | $-10 \rightarrow 9, 0 \rightarrow 15, 0 \rightarrow 8$ |
| Total reflections | 748 |
| Unique reflections | 692 |
| $ F_{\rm o} \ge 4\sigma_{\rm F}$ | 412 |
| Parameters | 64 |
| Final R (%) | 5 74 |
| Final S | 1 258 |
| | 1.230 |
| | |

$$R = \Sigma ||F_{o}| - |F_{c}||\Sigma|F_{o}|$$

$$S = \left[\sum w(|F_{o}| - |F_{c}|)^{2}/(m-n)\right]^{1/2}, \text{ for } m$$
observations and n parameters
$$w = 1/\left[\sigma(F_{o}^{2}) + (aP)^{2} + bP\right]$$

$$P = \left[2F_{c}^{2} + \max(F_{o}^{2}, 0)\right]/3$$

results, should be examined. In view of the fact that the phase is anhydrous, the composition of our Rb-feldspar indicates the incorporation of an Al(Al₃Si)O₈ component. The final refinement was carried out adopting a scheme of solid solution towards this component. It has been suggested tentatively that as the 'excess-Al-component' the Al(Al₃Si)O₈ end-member is introduced into anorthite megacrysts from island arc basalts (Kimata et al., 1995). A negative correlation between Al-excess and Rb is shown in Fig. 3, which implies the incorporation of this Al-excess end-member. The empirical formula for the Rbfeldspar in this study is thus estimated to be $Rb_{0.811} \square_{0.127}Al_{1.059}Si_{3.003}O_8$. Moreover, the H₂O molecules in Rb-feldspars have been interpreted as contributing to the processes of (Al,Si) ordering (Teertstra et al., 1998a,b). The deficiency of total wt.% in the EMP analyses (Table 1) suggests the existence of H_2O in the

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TABLE 3. Atomic parameters (upper) and their estimated standard deviations (lower) for Rb-feldspar.

| Site | x | у | Z. | U_{eq} | U_{11} | U_{22} | U ₃₃ | U ₂₃ | U_{13} | U_{12} (Å ²) |
|------------|--------|--------|--------|-------------------|----------|----------|-----------------|-----------------|----------|----------------------------|
| Rb | 0.2960 | 0.0000 | 0.1460 | 0.0454 | 0.0356 | 0.0641 | 0.0396 | 0.0000 | 0.0193 | 0.0000 |
| | 0.0004 | 0.0000 | 0.0005 | 0.0012 | 0.0017 | 0.0026 | 0.0021 | 0.0000 | 0.0015 | 0.0000 |
| T1 | 0.0106 | 0.1913 | 0.2223 | 0.0474 | 0.0451 | 0.0544 | 0.0478 | -0.0008 | 0.0250 | -0.0026 |
| | 0.0007 | 0.0005 | 0.0010 | 0.0017 | 0.0032 | 0.0042 | 0.0038 | 0.0031 | 0.0030 | 0.0030 |
| <i>T</i> 2 | 0.7235 | 0.1194 | 0.3446 | 0.0492 | 0.0480 | 0.0565 | 0.0505 | 0.0030 | 0.0285 | -0.0016 |
| | 0.0007 | 0.0005 | 0.0010 | 0.0017 | 0.0035 | 0.0040 | 0.0039 | 0.0033 | 0.0031 | 0.0031 |
| OA1 | 0.0000 | 0.1557 | 0.0000 | 0.0630 | 0.0500 | 0.0745 | 0.0652 | 0.0000 | 0.0262 | 0.0000 |
| | 0.0000 | 0.0020 | 0.0000 | 0.0066 | 0.0123 | 0.0174 | 0.0159 | 0.0000 | 0.0119 | 0.0000 |
| OA2 | 0.6662 | 0.0000 | 0.2834 | 0.0490 | 0.0611 | 0.0585 | 0.0388 | 0.0000 | 0.0324 | 0.0000 |
| | 0.0026 | 0.0000 | 0.0031 | 0.0054 | 0.0130 | 0.0139 | 0.0116 | 0.0000 | 0.0105 | 0.0000 |
| OB | 0.8311 | 0.1597 | 0.2245 | 0.0645 | 0.0455 | 0.0907 | 0.0595 | -0.0036 | 0.0252 | 0.0002 |
| | 0.0018 | 0.0015 | 0.0026 | 0.0050 | 0.0084 | 0.0140 | 0.0103 | 0.0097 | 0.0077 | 0.0088 |
| OC | 0.0444 | 0.3130 | 0.2585 | 0.0646 | 0.0827 | 0.0772 | 0.0413 | -0.0004 | 0.0341 | 0.0107 |
| | 0.0022 | 0.0014 | 0.0023 | 0.0049 | 0.0110 | 0.0120 | 0.0100 | 0.0088 | 0.0087 | 0.0104 |
| OD | 0.1692 | 0.1292 | 0.4026 | 0.0560 | 0.0617 | 0.0538 | 0.0671 | 0.0002 | 0.0416 | 0.0012 |
| | 0.0020 | 0.0012 | 0.0027 | 0.0042 | 0.0092 | 0.0100 | 0.0106 | 0.0085 | 0.0085 | 0.0083 |
| | | | | | | | | | | |

 $U_{\rm eq} = 1/3\Sigma U_{\rm ij}a_{\rm i}^*b_{\rm j}^*a_{\rm i}b_{\rm j}$

The anisotropic displacement factors are of the form: $-2\pi^2 [h^2 a^* U_{11} + \cdots + 2hka^* b U_{12}]$

Rb-feldspar supported by the IR spectrum data (Fig. 2).

Structural refinement

The SHELXL-97 program was used for crystal structure refinement of the Rb-feldspar. The structure was refined in the space group C2/m,



FIG. 3. Relationship between Rb in *M*-site and excess Al in synthetic Rb-feldspar.

and the starting atomic coordinates were taken from the structure of RbAlSi₃O₈ (Gasperin, 1971). Conventional refinements of diffraction data vielded reasonable interatomic distances and angles for the tetrahedral framework, but an agreement index (R) was very large (~10%) when all the reflections from $2-70^{\circ}2\theta$ were used. After omitting the reflections of higher angles $(2\theta > 50^\circ)$ because of the extreme weakness in these intensities, the R-value dropped drastically to 5.77% for Rb-feldspar. Moreover, after refining based on the chemical composition determined by EMPA, the final R factor achieved is 5.74%(Table 2), introducing the occupancies of 'excess-Al' at the M-site. Final positional and displacement parameters are given in Table 3 and selected interatomic distances and angles in Table 4.

Structure description

Examination of Fig. 4 shows that the calculated ellipsoids are not greatly distorted from spherical. Therefore no attempt was made to refine the structure using split atom positions, although no difference Fourier calculations were performed. Judging from the non-stoichiometry of the refined crystal, the final *R*-value (5.74%) is more reliable than that reported previously (7%) for disordered

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| <i>T</i> 1 –OA1 | 1.624 | (10) | | OA1- <i>T</i> 1-OB | 107.4 | (8) |
|---------------------|-------|------|-------|------------------------------------|-------|------|
| -OB | 1.646 | (16) | | OA1 - T1 - OC | 111.4 | (11) |
| -OC | 1.613 | (21) | | OA1-71-OD | 107.0 | (8) |
| -OD | 1.643 | (17) | | OB-T1-OC | 110.9 | (10) |
| Mean | 1.632 | | | OB-T1-OD | 111.1 | (9) |
| | | | | OC-T1-OD | 108.9 | (9) |
| | | | | Mean | 109.5 | |
| T2-OA2 | 1.636 | (9) | | OA2-72-OB | 110.4 | (10) |
| -OB | 1.626 | (17) | | OA2-72-OC | 105.7 | (10) |
| -OC | 1.675 | (19) | | OA2-72-OD | 109.3 | (9) |
| -OD | 1.641 | (19) | | OB-T2-OC | 108.2 | (8) |
| Mean | 1.645 | | | OB-72-OD | 111.9 | (8) |
| | | | | OC - <i>T</i> 2 - OD | 111.1 | (8) |
| | | | | Mean | 109.4 | |
| Rb – OA1 $\times 2$ | 3.106 | (17) | 0.204 | | | |
| -OA2 | 2.974 | (21) | 0.146 | | | |
| -OB × 2 | 3.168 | (18) | 0.174 | | | |
| $-OC \times 2$ | 3.140 | (18) | 0.186 | | | |
| $-OD \times 2$ | 3.049 | (15) | 0.240 | | | |
| Mean | 3.100 | Σ | 0.950 | | | |
| | | | | | | |

TABLE 4. Selected interatomic distances (Å), angles (°) and bond valences* (bv) for Rb-feldspar.

* Brown and Altermatt (1985)

Rb-feldspar (Gasperin, 1971). Rubidium-oxygen distances are slightly larger than those reported by Gasperin (1971), but no basic difference in topology has arisen between the two Rb-feldspars. The bond valence sum for the present Rb cation coordinated by nine O atoms is 0.950 bv, which is close to the Σ bv of 0.995 for previous Rb-feldspars (Gasperin, 1971). The lower bond valence sum than found in previous works may be consistent with the lower Rb contents, 'excess-Si' and H₂O molecules observed by EMPA and IR methods.

In nature, Rb-rich feldspars with the (Al,Si) ordered distribution are known as rubicline, analogous to microcline (Teertstra et al., 1998b, 1999a). In the present Rb-feldspar, the mean T1-O and T2-O distances exhibit a highly disordered (Al,Si) distribution (Table 4). The (Al,Si) distributions of the present Rb-feldspar calculated from T-O bond lengths (Kroll and Ribbe, 1983), namely Al/Si = 0.245/0.755 (T1 site) and Al/Si = 0.255/0.745 (T2 site), are similar in the ordering degree to those of the Rb-feldspar refined previously (Gasperin, 1971); Al/Si = 0.251/0.749 (T1 site), Al/Si = 0.249/0.751 (T2 site). However, there are significant differences in the cell parameters between the Rb-feldspar in the present work and that of Gasperin (Table 5). The cell parameters of our Rb-feldspar are entirely consistent with those reported by other recent studies (Voncken *et al.*, 1993; Koval'skii *et al.*, 2000). The differences between their chemical compositions may provide an explanation for the dissimilarity in cell parameters.

Geochemical implications

Most minerals in the Earth's upper mantle contain small amounts of structurally bound H. The OH concentration in each mineral species is variable, in some cases reflecting the geological environment of mineral formation (Bell and Rossman, 1992). Reported analyses of feldspars in nature often include H_2O molecules or $(H_3O)^+$ ions entering the M site in the feldspar structure (Smith, 1983). In particular, large cations such as K, Rb, Sr, Cs and Ba are frequently contained in feldspar structures capable of accompanying H₂O molecules (Hofmeister and Rossman, 1985; Beran, 1986; Teertstra et al., 1998a,b,c). The large non-tetrahedral site, normally occupied by K for sanidine, is well-suited to the site which probably holds the water (Beran, 1986). The incorporation of H₂O molecules into Rb-feldspar is ascribed to the \Box Si₄O₈ substitution, because of the generation of a large vacancy in the *M*-site.

The early data suggesting that substitution of Rb for K restricts the degree of (Al,Si) ordering

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FIG. 4. ORTEP representation of the Rb-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 Rb to the framework is not shown.

from sanidine to microcline was reaffirmed by Afonina *et al.*, (1979). Smith (1983) suggested that although most of the K-feldspars with high Ba, Rb and Cs are not fully ordered, a few are strongly ordered, perhaps because of late-stage processes. The present RbAlSi₃O₈ feldspar with

| TABLE 5. Unit-cell parameters of the synthetic Rb-feldspar in comparison with other Rt | b-feldspar |
|--|------------|
|--|------------|

| a (Å) | <i>b</i> (Å) | <i>c</i> (Å) | β (°) | $V(\text{\AA}^3)$ | Reference |
|----------|--------------|--------------|------------|-------------------|-----------|
| 8.839(2) | 13.035(2) | 7.175(2) | 116.11(1) | 742.3(3) | 1 |
| 8.837(2) | 13.035(3) | 7.187(1) | 116.27(1) | 742.4(2) | 2 |
| 8.841(1) | 13.036(1) | 7.195(1) | 116.208(8) | 743.5(3) | 3 |
| 8.839(1) | 13.034(1) | 7.182(1) | 116.29(1) | 741.8(2) | 4 |
| 8.834(4) | 13.042(5) | 7.195(3) | 116.42(3) | 742.38(1) | 5 |
| 8.820 | 12.992 | 7.161 | 116.24 | 736.0 | 6 |
| 8.844 | 13.044 | 7.190 | 116.35 | 743.3 | 7 |
| 8.842 | 13.043 | 7.189 | 116.32 | 743.2 | 7 |

1: this study; 2: Voncken *et al.* (1993); 3: Koval'skii *et al.* (2000); 4: Bruno and Pentinghaus (1974);

5: Ghelis and Gasperin (1970); 6: Gasperin (1971); 7: Henderson (1978)

the (Al,Si) disordered distribution has been synthesized hydrothermally from the low albite with the (Al,Si) ordered distribution, Meanwhile, the original view has been put forward that diffusion of Rb⁺ and nucleation in the $\Box Si_4O_8$ rich microcline leads to formation of rubicline with the (Al,Si) ordered distribution in the granitic pegmatite (Teertstra *et al.*, 1998*b*). Therefore it is unclear from the results above how Rb can retard the ordering process in the feldspar framework (Smith, 1983; Teertstra *et al.*, 1998*b*).

This study has two geochemical implications: (1) synthetic and natural feldspars composed of the larger *M*-cations tend to incorporate the water, $\Box Si_4O_8$ end-members and excess Al; and (2) confirmation of synthetic RbAlSi₃O₈ with (Al,Si) disordered distribution and discovery of (Al,Si) ordered rubicline in nature mean that both the (Al,Si) ordered and disordered frameworks of feldspars can accommodate the Rb cation.

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