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A RE-EXAMINATION OF THE PELLOTSALO MICROCLINE: MINERALOGICAL IMPLICATIONS AND GENETIC CONSIDERATIONS

ACHILLE BLASI AND CARLA DE POL BLASI
Dipartimento di Scienze della Terra, Università degli Studi, Via Botticelli 23, 20133 Milano, Italy

PIER FRANCESCO ZANAZZI
Dipartimento di Scienze della Terra, Università di Perugia, Piazza Università, 06100 Perugia, Italy

ABSTRACT

A largely perthitic intergrowth from a granitic pegmatite in the island of Pellotsalo, Lake Ladoga, U.S.S.R., has been re-investigated. The specimen is from the same crystal used by Brown & Bailey (1964) to isolate their original Pellotsalo microcline. Microprobe analyses gave $Or_{93.62}Ab_{6.10}An_{0.05}Cn_{0.02}Rbf_{0.21}$(mol.%) for the K-rich phase and $Or_{1.05}Ab_{98.07}An_{0.88}$ (mol.%) for the Na-rich phase. The crystal structure of the K-rich phase was refined to a value of *R* of 0.027 for 1232 observed diffraction-maxima. The new structural data are very similar to those of the Prilep (Strob 1983) and Pikes Peak (Blasi *et al.* 1984b) specimens and provide much the same response as the metric properties. On the assumption of complete Si,Al order, these specimens give mean Al–O and Si–O distances equal to 1.738 and 1.614 Å, respectively. These values are slightly different from those found in Na-rich feldspar and should be used for converting mean *T*–O distances to Al contents in K-rich feldspar alone. The contrasting genetic interpretations formulated concerning the Pellotsalo feldspar during this century are due to the ambiguous occurrence of irregular patches of cross-hatching in the K-rich phase. The latter shows no evidence of monoclinic ancestry in single-crystal X-ray photographs, but weak streaks from the coexisting Na-rich phase may be interpreted in favor of an incipient M-twinning as the result of exsolution in a monoclinic environment. The implication of M-twinning, the high Na-content of the bulk composition ($Or_{72}Ab_{27}An_1$ mol.%: Goldsmith & Laves 1961), the moderate enrichment in Rb and the low concentration of Ba in the K-rich phase suggest that the Pellotsalo microperthite formed at a temperature just above that of the $C2/m \rightarrow C\bar{1}$ inversion.

Keywords: alkali feldspar, low microcline, electron-microprobe analysis, metric and structural properties, mean Al–O and Si–O distances, genetic considerations, island of Pellotsalo, Lake Ladoga, U.S.S.R.

SOMMAIRE

Un feldspath à intercroissance perthitique prédominante d'une pegmatite granitique de l'île de Pellotsalo, lac Ladoga (URSS), a fait l'objet d'une nouvelle étude. Nous avons utilisé un échantillon provenant du même cristal duquel Brown et Bailey (1964) ont prélevé leur microcline de Pellotsalo. Les analyses à la microsonde ont donné $Or_{93.62}Ab_{6.10}An_{0.05}Cn_{0.02}Rbf_{0.21}$ (base molaire) pour la phase potassique et $Or_{1.05}Ab_{98.07}An_{0.88}$ pour la phase sodique. La structure cristalline de la phase potassique a été affinée à un résidu *R* de 0.027 pour 1232 réflexions observées. Les nouvelles données structurales ressemblent beaucoup à celles des échantillons de Prilep (Strob 1983) et Pikes Peak (Blasi *et al.* 1984b) et montrent les mêmes tendances que les propriétés métriques. En supposant un degré d'ordre Al,Si parfait, ces échantillons indiquent des longueurs moyennes des liaisons Al–O et Si–O égales à 1.738 et 1.614 Å, respectivement. Ces valeurs diffèrent légèrement de celles qui caractérisent l'albite, et devraient être utilisées pour établir la conversion des longueurs de liaison *T*–O à la proportion d'aluminium dans les échantillons de feldspath potassique seulement. Les interprétations pétrogénétiques contradictoires formulées à propos du microcline de Pellotsalo depuis le début du siècle sont dues à la présence ambiguë de domaines à maclage quadrillé en taches irrégulières dans la phase potassique. Celle-ci ne montre aucune indication d'un précurseur monoclinique dans les clichés de rayons X sur cristal unique; on peut interpréter les faibles rayures dues à la phase sodique coexistante comme indications d'un début de maclage de type M résultant de l'exsolution dans un milieu monoclinique. Le maclage M, la teneur élevée en sodium de la composition globale ($Or_{72}Ab_{27}An_1$: Goldsmith et Laves 1961), l'enrichissement moyen en rubidium, et la faible concentration de baryum dans la phase potassique font penser que la microperthite de Pellotsalo s'est formée à une température légèrement au dessus de l'inversion $C2m/ \rightarrow C\bar{1}$.

(Traduit par la Rédaction)

Mots-clés: feldspath alcalin, microcline ordonné, analyse à la microsonde électronique, propriétés métriques et structurales, distances Al–O et Si–O moyennes, considérations génétiques, île de Pellotsalo, lac Ladoga, URSS.

INTRODUCTION

What is currently known as Pellotsalo microcline is the K-rich phase of a largely perthitic intergrowth from a granite pegmatite body in the island of Pellotsalo, Sortavalan Pit, near the northern coast of Lake Ladoga (westernmost U.S.S.R.). The occurrence of this feldspar has been known in the geological and mineralogical literature since the end of the last century.

The crystal structure of the K-rich phase of the Pellotsalo perthite was refined by Brown & Bailey (1964). Their data are consistent with the extreme state of Si,Al order attainable in microcline and are still considered very good today (*cf.* Blasi *et al.* 1984b).

Results of a structure refinement performed by Finney & Bailey (1964) on an authigenic maximum microcline from the Pontiskalk limestone, Switzerland, indicate slightly less order than in the Pellotsalo specimen. Blasi *et al.* (1984b) showed that these results contain a high number of significant abnormalities in interatomic distances and angles.

Three new structure-refinements of presumably fully ordered microcline have recently become available (Prilep, Yugoslavia: Strob 1983; 7813A and 7813B from the Pikes Peak batholith, Colorado: Blasi *et al.* 1984b). On the basis of their metric and structural properties, these three specimens appear to be very similar to each other.

The degree of Si,Al order estimated from cell constants seems to be somewhat higher in these three specimens than in the Pellotsalo microcline. Yet, the latter appears to be the most ordered specimen on the basis of mean *T*–O distances. This contradiction is accompanied in the Pellotsalo specimen by an as yet unresolved anomalous discrepancy between the $\Delta(bc)$ and $\Delta(b^*c^*)$ values, which was first observed by Blasi (1980) and then reconsidered by Blasi *et al.* (1984b).

Knowledge of the exact nature of fully ordered microcline is a key feature in understanding feldspar mineralogy and unravelling petrological problems. In this light, a re-investigation of the Pellotsalo microperthite was undertaken, to determine the composition of the individual components of the intergrowth and to derive the metric and structural properties of the K-rich phase. A preliminary account of these results has already been given by Blasi *et al.* (1986). Our aim is to assess the mineralogical implications of the more accurately and precisely known mean Al–O and Si–O distances in fully ordered K-rich feldspar. In addition, the present data and those of earlier investigators will be used to clarify the contrasting genetic interpretations that have been put forward regarding the Pellotsalo specimen.

HISTORICAL NOTES

The first description of the Pellotsalo microperthite was given by Ramsay & Zilliacus (1897, p. 59 and footnote thereto). Further data were reported by Mäkinen (1913, p. 60-61 and 63-64) and Eskola (1951, p. 39-40, Figs. 1 and 2 in Plate I). Goldsmith & Laves (1954, 1961), Hafner & Laves (1957), and Laves & Hafner (1962) studied material provided by P. Eskola. J.R. Goldsmith sent S.W. Bailey a thumbnail-size single crystal of the original specimen; a cleavage fragment of the K-rich phase was used in structure refinement by Brown & Bailey (1964; see also Brown 1962). Smith (1974b) published two microphotographs (his Fig. 18–31) and electron-microprobe data (his Table 19–5) obtained from a specimen provided by J.R. Goldsmith. Mason (1982) carried out electron- and ion-microprobe analyses of the components of the Pellotsalo perthite.

The material investigated here was kindly supplied by S.W. Bailey and comes from the same crystal employed by Brown & Bailey (1964) to isolate the fragment that they used in structure refinement.

MATERIAL INVESTIGATED

The optical micrographs of the Pellotsalo perthite published by Eskola (1951), Goldsmith & Laves (1954, Figs. 15a, 15b), and Smith (1974b) are similar. The predominant K-rich phase is microcline, which is largely untwinned, but subordinately shows irregular patches of cross-hatched or albite twinning. The Na-rich phase consists of subparallel stringers of albite, which are usually somewhat coarse and show polysynthetic albite twinning.

A number of cleavage fragments of the K-rich phase were isolated and subjected to single-crystal X-ray photography [*Y*-axis oscillation technique in the special orientation of Smith & MacKenzie (1955) and precession method about the *X* and *Z* axes with *Y** parallel to the dial axis].

The specimen chosen for subsequent cell-constant and structure refinements is a transparent, rather well-formed cleavage fragment showing {010} dominant over {001}. The dimensions of the crystal are smaller than those of the fragment used in structure refinement by Brown & Bailey (1964): $0.04 \times 0.14 \times 0.18$ *versus* $0.15 \times 0.20 \times 0.25$ mm. The specimen chosen consists of a dominant K-rich phase and very minor Na-rich phase. The K-rich phase shows sharp spots, some of which are accompanied by short streaks lying on curves of constant θ. This may be the result of structural continuity of a very small quantity of K-rich feldspar material rotated from the dominant unit. The Na-rich phase exhibits very rare weak streaks, whose positions would seem to be consistent with a strongly unbalanced M-twinning of low albite.

The feldspar material available was too sparse for X-ray powder patterns. However, small fragments could be selected for electron-microprobe investigation.

CHEMICAL COMPOSITION

The fragments were analyzed by wavelength dispersion on an ARL–SEMQ electron microprobe using TAP, ADP, PET, and LiF monochromators. Wavelength profiles for each X-ray line were carefully measured in all the standards and the unknown in order to select appropriate background-positions. The raw spectrometer-data were corrected and reduced on an on-line PDP 11/23 computer using the MAGIC IV program of Colby (1971).

An initial series of microprobe analyses was

TABLE 1. CHEMICAL COMPOSITION DERIVED BY ELECTRON-MICROPROBE ANALYSIS OF COMPONENTS OF THE PELLOTSALO PERTHITE

	K-rich phase						Na-rich phase		
	1	2	3	4			5	6	
	wt.%	wt.%	wt.%	Atoms (O=8)			wt.%	Atoms (O=8)	
SiO_2	64.83	64.87	64.85	Si	3.000	SiO_2	68.29	Si	2.994
Al_2O_3	18.35	18.32	18.34	Al	1.000	Al_2O_3	19.35	Al	1.000
CaO	0.02	0.00	0.01	Σp	4.000	CaO	0.19	Σp	3.994
Na_2O	0.70	0.66	0.68	Na	0.061	Na_2O	11.71	Na	0.995
K_2O	15.85	15.85	15.85	K	0.935	K_2O	0.19	K	0.011
	Σt 99.75	Σp 99.70	Σp 99.73	Rb	0.002		Σp 99.73	Ca	0.009
FeO		0.00	0.00	Σp	0.998	FeO	0.00	Σp	1.015
SrO		0.00	0.00	Σt	4.998	SrO	0.00	Σt	5.009
BaO		0.01	0.01	End-member mol.%		BaO	0.00	End-member mol.%	
Rb_2O		0.07	0.07			Rb_2O	0.00		
		Σt 99.78	Σt 99.81	Or	93.62		Σt 99.73	Or	1.05
				Ab	6.10			Ab	98.07
				An	0.05			An	0.88
				Cn	0.02				
				Rbf	0.21				

Σp and Σt denote partial and total sum, respectively.

1 Standards used were orthoclase PSU Or-1A (Ingamells 1978) for Si, Al, and K; albite, Amelia, Virginia, for Na; diopside, Natural Bridge, New York, USNM 117733 (Jarosewich *et al.* 1980) for Ca.

2 Standards used were those listed in footnote 1 for Si, Al, K, and Ca; albite, Avigliana, Piemonte, Italy, for Na; olivine (Fo_{90}), San Carlos, Gila Co., Arizona, USNM 111312/444 (Jarosewich *et al.* 1980) for Fe; synthetic celestite for Sr; synthetic celsian for Ba; $RbMnF_3$ for Rb.

3 Adopted composition.

4 Chemical formula and end-member compositions were calculated using the data in column 3.

5 Standards used were those listed in footnote 2.

6 Chemical formula and end-member compositions were calculated using the data in column 5.

performed in order to determine K, Na, Ca, Al and Si. The following operating conditions were used: accelerating voltage 15 kV, emission current 150 μA, sample current standardized on brass 0.010 μA, beam diameter 15 μm. The average of 10 of these analytical results is reported in column 1 of Table 1.

A second series of microprobe analyses was performed to determine Ba, Sr, Rb and Fe, along with K, Na, Ca, Al and Si. The following analytical conditions were employed: accelerating voltage 25 kV, emission current 150 μA, sample current standardized on brass 0.030 μA, beam diameter 20 μA. The average of 10 of these analytical results is presented in column 2 of Table 1.

The composition adopted for the Pellotsalo microcline is reported in column 3 of Table 1 and represents the average of the data given in columns 1 and 2. The relevant chemical formula and end-member compositions are shown in column 4. The analytical data reveal a low amount of Na and virtual absence of Ca. In agreement with these results, the composition of a Pellotsalo microcline was found to be $Or_{92.6}Ab_{7.4}An_{0.0}$ mol.% by Smith (1974b, Table 19–5, original data in wt.%) using wavelength-dispersion electron-microprobe techniques and $Or_{95}Ab_5An_0$ mol.% by Mason (1982, Table II) employing energy-dispersion electron-microprobe methods. The minor-element concentrations presented in Table 1 are consistent with those determined by Mason (1982, Table II) using ion-microprobe techniques.

During the second round of microprobe analyses, systematic scanning with the electron beam showed that almost all the bright-blue homogeneous luminescence of the dominant K-rich phase disappeared suddenly in small well-delimited areas. Microprobe analyses of these areas showed that they were made of the Na-rich phase. The average of 4 of these analytical results is given in column 5 of Table 1. The chemical formula and end-member compositions are shown in column 6. These results indicate that the Na-rich phase is very pure. In accordance with these data, the composition of the Na-rich component of a Pellotsalo microperthite was found to be $Or_{0.0}Ab_{99.1}An_{0.9}$ mol.% in the core and $Or_{0.3}Ab_{98.6}An_{1.1}$ mol.% in the rim by Smith (1974b, Table 19–5, original data in wt.%) using wavelength-dispersion electron-microprobe methods, and $Or_{1.3}Ab_{97.7}An_{1.0}$ mol.%, on average, by Mason (1982, Table II) utilizing energy-dispersion electron-microprobe techniques.

The bulk composition of a Pellotsalo microperthite determined by spectrochemical analysis was reported to be $Or_{72}Ab_{27}An_1$ mol.% by Goldsmith & Laves (1961, Table III, original data in wt.%). The importance of this will be discussed later.

INFERENCES FROM METRIC PROPERTIES

General statement

The values of 2θ angles for cell-constant refinement were collected in the 20–50° 2θ range on a Philips PW1100 four-circle, computer-controlled, single-crystal diffractometer using graphite-monochromatized $CuK\alpha$ radiation. Additional experimental details are given by Blasi *et al.* (1981). Refined cell-constants and related indicators are listed in Tables 2 and 3, respectively, along with the corresponding data for the specimen studied by Brown & Bailey (1964).

TABLE 2. DIRECT AND RECIPROCAL CELL-CONSTANTS FOR THE PELLOTSALO MICROCLINE

#	a, Å	b, Å	c, Å	α, °	β, °	γ, °	V, Å³	SQRSG ×10³, Å⁻²§	N†
	a^*, Å⁻¹	b^*, Å⁻¹	c^*, Å⁻¹	α*, °	β*, °	γ*, °	$V^* \times 10^5$, Å⁻³		
1 This work¶									
	8.5714(3)	12.9646(4)	7.2217(2)	90.636(3)	115.949(2)	87.679(3)	720.99(3)	0.03	40
	0.129850(4)	0.077199(2)	0.154001(4)	90.423(3)	64.055(2)	92.272(3)	138.698		
2 Brown & Bailey (1964)+									
	8.560(4)	12.964(7)	7.215(3)	90.656(80)	115.838(80)	87.704(80)	720.0		
	0.1299	0.0772	0.1540	90.383	64.167	92.233	138.89		
3 Brown & Bailey (1964) modified≡									
	8.567	12.964	7.221	90.660	115.935	87.703	720.6		
	0.1299	0.0772	0.1540	90.383	64.070	92.233	138.77		

Estimated standard errors (1σ) are given in parentheses and refer to the last decimal place.

† Number of diffractions used in cell refinement.

§ Estimated standard error of unit-weight observation of Q, based on refinement of six parameters.

¶ Cell constants were refined with the LCLSQ program of Burnham (1962) slightly modified by Blasi (1979) and Blasi & De Pol Blasi (1980). Unit weight and wavelength λ(Cu$K\alpha$) = 1.54178 Å were used in each observation.

+ Direct cell-constants were re-calculated from reciprocal cell-constants determined by Brown & Bailey (1964) using the θ-method of Weisz *et al.* (1948). The number of figures for direct cell-angles is consistent with that for reciprocal cell-angles converted from degrees and minutes to degrees and decimals without any rounding. The values of α and β were reported by Brown & Bailey (1964) to be 90° 39' (90.650°) and 115° 50' (115.833°), respectively.

≡ Direct cell-constants were calculated from reciprocal cell-constants of Brown & Bailey (1964) replacing β* = 64.167° by β* = 64.070°. The number of figures is in conformity with that given for data set #2.

TABLE 3. STRUCTURAL INDICATORS, TETRAHEDRAL SITE-OCCUPANCIES, STRAIN INDICES, AND MOLE FRACTIONS OF $KAlSi_3O_8$ ESTIMATED FROM CELL CONSTANTS FOR THE PELLOTSALO MICROCLINE

#	Δ(bc) §	Δ(αγ) §	t1o §	t1m §	t2 §	$Or(b^*c^*)$§	Δa, Å¶	N_{Or}† from V
	Δ(b^*c^*)	Δ(α*γ*)	t1o*	t1m*	t2*			from a
1 This work								
	0.998(2)	0.988(1)	0.993(1)	0.005(1)	0.001(1)	1.001(1)	-0.023	0.954
	0.999(2)	0.986(1)	0.993(1)	0.006(1)	0.001(1)			0.949
2 Brown & Bailey (1964)								
	0.951(28)	0.977(34)	0.964(22)	-0.013(22)	0.024(14)	1.000	0.010	0.929
	1.000	0.976	0.988	0.012	0.000			0.922
3 Brown & Bailey (1964) modified+								
	0.995	0.978	0.986	0.009	0.003	1.000	-0.021	0.944
	1.000	0.976	0.988	0.012	0.000			0.938

Estimated standard errors (1σ) are given in parentheses and refer to the last decimal place.

† Calculated from the relevant quadratic least-squares fits given by Blasi & De Pol Blasi (1980) for the microcline-series data of Hovis & Peckins (1978).

§ Principal quantities and standard errors were calculated following the procedures described by Blasi (1977, 1979) and Blasi & De Pol Blasi (1980). The cell constants proposed by Smith (1974a) for the alkali feldspar end-members were involved in calculations.

¶ Determined graphically following the procedure indicated by Stewart & Wright (1974).

+ See footnote ≡ to Table 2.

Taken at face value, data sets 1 and 2 in Table 2 appear to be somewhat different: the direct cell-constants show the most significant discrepancies in a, c, β, and V, whereas the reciprocal cell-constants differ mainly in β* and V^*.

As already indicated, the specimen of Brown & Bailey (1964) is affected by an anomalous discrepancy between the values of Δ(bc) and Δ(b^*c^*). In fact, the difference Δ(bc) - Δ (b^*c^*) obtainable from data set 2 in Table 3 amounts to -0.049, which is well outside the limits predicted by Blasi (1980) for specimens of low microcline.

Some error in the metric parameters of Brown & Bailey (1964) was therefore suspected. The most probable source of bias is in angle β*. Its value, 64.167° (Table 2), is tangibly higher than that of other specimens of low microcline (usually ranges between ~64.05 and ~64.09°). For any β* in this range, the reciprocal cell-constants of Brown & Bailey (1964) give rise to new values of a, c, β, V, and V^* that agree well with those for the specimen investigated in this paper. This modification of the β* angle causes Δ(bc) to increase and the absolute value of the difference Δ(bc) - Δ(b^*c^*) to drop within the limits predicted by Blasi (1980). In addition, the change in β* renders the values of t1o, t1m, t2, Δa, and N_{Or} in the microcline of Brown & Bailey (1964) remarkably similar to those obtained for the specimen investigated here. For the sake of illustration, Tables 2 and 3 show results obtained by using an intermediate β* value of 64.07°, which renders the difference Δ(bc) - Δ(b^*c^*) equal to -0.005.

Structural state

The values of [Δ(bc) + Δ(b^*c^*)]/2 and [Δ(αγ) + Δ(α*γ*)]/2 as well as those of (t1o + t1o*)/2, (t1m + t1m*)/2, and (t2 + t2*)/2 (#1, Table 3) suggest that the Pellotsalo feldspar is likely to be slightly less ordered than the Prilep microcline investigated by Strob (1983) and the two specimens of Pikes Peak microcline studied by Blasi *et al.* (1984b).

Composition of K-rich phase

The composition calculated from V for the Pellotsalo microcline (#1, Table 3) is slightly more K-rich than that obtained by microprobe measurements (Table 1). Similar behavior was found in the Pikes Peak microcline by Blasi *et al.* (1984b), who proposed that the volume excited by the electron beam probably includes small amounts of a Na-rich phase. The scattering factor for the M position in the specimen investigated here has consequently been assumed to be $0.95f_K + 0.05f_{Na}$ on the basis of the value of $N_{Or} = 0.95$ obtained from V (#1, Table 3). By contrast, the linear absorption-coefficient has been calculated as $\mu(\text{Mo}K\alpha) = 13.3 \text{ cm}^{-1}$ using the less potassic composition determined by microprobe analysis (Table 1).

On the basis of the composition estimated from V, the Pellotsalo feldspar appears to be ~2 mol.% Or less potassic than the Prilep (Strob 1983) and Pikes Peak (Blasi *et al.* 1984b) specimens.

Lattice strain

The a^* (#1, Table 2) *versus* $\text{Or}(b^*c^*)$ (#1, Table 3) relationship introduced by Smith (1974a, Fig. 7-27), as well as the values of the Δa indicator (#1, Table 3) proposed by Stewart & Wright (1974), indicate that lattice strain is absent in the Pellotsalo specimen. This is also confirmed by the small negative difference between the values of $N_{Or}(a)$ and $N_{Or}(V)$ (#1, Table 3)).

As with the Prilep (Strob 1983) and Pikes Peak (Blasi *et al.* 1984b) examples, the Pellotsalo specimen shows a slight tendency to reverse strain. As discussed by Blasi *et al.* (1984a, p. 431-432), this is not uncommon in K-rich feldspar and is worth further investigation.

INFERENCES FROM STRUCTURAL PROPERTIES

General statement

The diffraction intensities for the Pellotsalo microcline were collected on the same Philips PW1100 instrument employed to obtain the 2θ values used in cell-constant refinement. The measurements were done with graphite-monochromatized Mo$K\alpha$ radiation ($\lambda = 0.71069$ Å) in the range $4 \leq 2\theta \leq 60°$. Stationary background-counts were measured for 5 s on each side of the peaks. Three standard diffraction-maxima were measured after every 180 min in order to check mechanical alignment and electronic stability. These measurements oscillated within 2% throughout data collection. The raw intensity data were corrected for Lorentz and polarization effects. Despite the low linear absorption-coefficient [$\mu(\text{Mo}K\alpha) = 13.3 \text{ cm}^{-1}$; see previous section], a semiempirical correction for absorption was applied using the procedure developed by North *et al.* (1968). The refinement of the structure was performed following the procedure described by Blasi *et al.* (1981) by means of the full-matrix least-squares program SHELX-76 written by Sheldrick (1976). As indicated in the previous section, the scattering factor for the M position was assumed to be $0.95f_K + 0.05f_{Na}$. Further details of the experimental and structure-refinement parameters are given in Table 4. Fractional atomic co-ordinates, equivalent isotropic temperature-factors, anisotropic temperature-factors, and magnitudes and orientation of the thermal ellipsoid for the M atom are presented in Table 5. Polyhedral interatomic distances and angles are given in Table 6. The observed and calculated structure-factors can be obtained from the authors.

Accuracy and precision of results

The final R factor reported in Table 4 and the standard errors in the data presented in Tables 5 and 6 indicate that the quality of the structure refinement in this paper is significantly better than in that of Brown & Bailey (1964). The R factor in Table 4 and the standard errors in Tables 5 and 6 are virtually indistinguishable from those obtained by Blasi *et al.* (1984b) for their two Pikes Peak specimens 7813A and 7813B. No comparison is possible with the Prilep microcline of Strob (1983) because of the lack of pertinent data. The only structural data available on the latter specimen are those covering mean T–O distances, which have been reported by Kroll & Ribbe (1983) and Ribbe (1984).

Fractional atomic co-ordinates

The positional parameters listed in Table 5 are somewhat different from those obtained by Brown & Bailey (1964) for their Pellotsalo microcline. The most significant discrepancies lie mainly in the x coordinate for the $T1o$, OBo, OCm, and ODo atoms and the z co-ordinate for the $T1m$, OBm, OCm, and ODm atoms. Comparison of the atomic co-ordinates

TABLE 4. ADDITIONAL INFORMATION ON INTENSITY COLLECTION AND STRUCTURE REFINEMENT FOR THE PELLOTSALO MICROCLINE

Scan mode	ω-2θ
Scan speed	0.72° 2θ/min
Scan width	3.4° 2θ
Range of transmission factors	0.99-0.88
Collected diffractions	3991 ($\pm h, \pm k, \pm l$)
Merging R for equivalent diffractions	0.021 (on I)
Independent diffractions	2137
Observed diffractions	1232 with $I \geq 3\sigma(I)$
Number of variables	118
R	0.027
R_w	0.030
Weighting scheme	$w = 1/[\sigma^2(F_o) + 0.003F_o^2]$

TABLE 5. FRACTIONAL ATOMIC CO-ORDINATES, EQUIVALENT ISOTROPIC TEMPERATURE-FACTORS, AND ANISOTROPIC TEMPERATURE-FACTORS FOR THE PELLOTSALO MICROCLINE

Atom	x	y	z	Beq†	U_{11}§	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
M	0.2826(1)	0.9928(1)	0.1367(1)	1.64	145(4)	228(4)	236(5)	5(3)	70(3)	0(3)
T1o	0.0100(1)	0.1877(1)	0.2170(2)	0.63	92(4)	77(4)	77(5)	-19(3)	40(4)	8(4)
T1m	0.0098(1)	0.8196(1)	0.2323(1)	0.59	92(4)	78(4)	66(4)	7(3)	45(3)	7(3)
T2o	0.7111(1)	0.1204(1)	0.3401(1)	0.57	84(4)	56(4)	83(4)	-11(3)	42(3)	8(3)
T2m	0.7057(1)	0.8856(1)	0.3505(1)	0.59	77(4)	66(4)	86(4)	-2(3)	40(3)	9(3)
OA1	0.0007(3)	0.1448(2)	0.9829(4)	1.01	180(12)	134(11)	85(11)	-8(9)	70(9)	22(9)
OA2	0.6365(3)	0.0055(2)	0.2857(4)	0.82	106(10)	58(10)	131(12)	6(8)	36(9)	8(8)
OBo	0.8212(3)	0.1477(2)	0.2199(4)	1.25	139(12)	190(13)	187(13)	-48(9)	105(10)	2(10)
OBm	0.8319(3)	0.8573(2)	0.2401(4)	1.29	147(12)	203(13)	179(14)	45(10)	110(10)	17(11)
OCo	0.0353(3)	0.3200(2)	0.2511(4)	0.95	110(11)	105(11)	145(12)	-34(8)	51(9)	0(9)
OCm	0.0381(3)	0.6955(2)	0.2702(4)	0.89	122(10)	98(11)	140(12)	18(8)	79(9)	23(9)
ODo	0.1903(3)	0.1229(2)	0.4055(4)	1.10	162(12)	134(12)	93(12)	19(9)	32(9)	31(9)
ODm	0.1754(3)	0.8745(2)	0.4118(4)	1.17	157(11)	157(12)	93(12)	-47(9)	15(10)	8(9)

r.m.s. components of thermal displacement along principal axes (r) and thermal-ellipsoid orientation for M

r	r.m.s. displacement (Å)	Angle (°) with respect to X	Y	Z
1	0.120	156	83	86
2	0.152	85	167	100
3	0.159	67	79	169

Estimated standard errors (1σ) are given in parentheses and refer to the last decimal place.

† Beq values are expressed in Å² and were calculated from the anisotropic temperature-factors using the formulation of Hamilton (1959).

§ U_{ij} values (x10⁴) are expressed in Å² and appear in the anisotropic temperature-factor as: $\exp[-2\pi^2(h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33}+2hka^*b^*U_{12}+2hla^*c^*U_{13}+2klb^*c^*U_{23})]$.

TABLE 6. INTERATOMIC DISTANCES AND ANGLES FOR THE PELLOTSALO MICROCLINE

	T-O distances		O-O distances	O-T-O angles		T-O distances		O-O distances	O-T-O angles
T1o tetrahedron					T1m tetrahedron				
T1o-OA1	1.743(3)	OA1-OBo	2.756(5)	105.1(1)	T1m-OA1	1.590(3)	OA1-OBm	2.583(5)	107.8(1)
-OBo	1.729(3)	-OCo	2.908(5)	113.2(1)	-OBm	1.607(2)	-OCm	2.689(5)	113.6(1)
-OCo	1.739(3)	-ODo	2.771(5)	105.4(1)	-OCm	1.625(2)	-ODm	2.591(5)	107.3(1)
-ODo	1.740(3)	OBo-OCo	2.893(5)	113.1(1)	-ODm	1.629(2)	OBm-OCm	2.635(5)	109.3(1)
Mean	1.738(1)	-ODo	2.850(5)	110.6(1)	Mean	1.613(1)	-ODm	2.666(5)	111.0(1)
		OCo-ODo	2.834(5)	109.1(1)			OCm-ODm	2.633(5)	108.0(1)
		Mean	2.835	109.4			Mean	2.633	109.5
T2o tetrahedron					T2m tetrahedron				
T2o-OA2	1.620(2)	OA2-OBo	2.654(5)	111.7(1)	T2m-OA2	1.639(2)	OA2-OBm	2.610(5)	106.0(1)
-OBo	1.587(3)	-OCm	2.559(5)	104.1(1)	-OBm	1.630(3)	-OCo	2.562(5)	104.9(1)
-OCm	1.625(3)	-ODm	2.614(5)	107.4(1)	-OCo	1.594(3)	-ODo	2.633(5)	109.1(1)
-ODm	1.624(3)	OBo-OCm	2.654(5)	111.5(1)	-ODo	1.592(3)	OBm-OCo	2.642(5)	110.1(1)
Mean	1.614(1)	-ODm	2.666(5)	112.2(1)	Mean	1.614(1)	-ODo	2.657(5)	111.1(1)
		OCm-ODm	2.657(5)	109.7(1)			OCo-ODo	2.688(5)	115.1(1)
		Mean	2.634	109.4			Mean	2.632	109.4

	M-O distances			T-O-T angles
M-OA1	2.876(2)		T1o-OA1-T1m	144.5(1)
-OA1	2.882(3)		T2o-OA2-T2m	138.6(1)
-OA2	2.751(2)		T1o-OBo-T2o	151.0(1)
-OBo	2.961(3)		T1m-OBm-T2m	155.5(1)
-OBm	3.126(3)		T1o-OCo-T2m	131.1(1)
-OCo	2.912(3)		T1m-OCm-T2o	131.2(1)
-OCm	3.346(3)		T1o-ODo-T2m	140.2(1)
-ODo	2.898(3)		T1m-ODm-T2o	142.6(1)
-ODm	2.986(3)		Mean	141.8
Mean	2.971	(CN=9)		

Distances are expressed in Å and angles in degrees. Estimated standard errors (1σ) are given in parentheses and refer to the last decimal place. Values of σ in mean T-O distances were calculated according to the Law of Propagation of Errors (see Blasi 1977) assuming that (a) individual T-O distances can be considered as uncorrelated, and (b) co-variance terms can be neglected.

in Table 5 with the corresponding data for the two Pikes Peak specimens of Blasi *et al.* (1984b) shows that the former are rather similar to those of 7813A and virtually indistinguishable from those of 7813B.

Temperature factors

Brown & Bailey (1964) determined isotropic B values for all atoms, but anisotropic B values only for the M atom. These data were obtained using scattering factors for ionized atoms (Brown & Bailey 1964; see also Finney & Bailey 1964, p. 417). The anisotropic temperature-factors presented in Table 5 were obtained using neutral-atom scattering-factors for reasons of uniformity with the structure refinements of the two specimens of Pikes Peak microcline investigated by Blasi *et al.* (1984b). When using scattering factors for ionized rather than neutral atoms, the values of the thermal parameters can change appreciably, whereas the shape and orientation of the displacement ellipsoids remain virtually unchanged. For that reason, the temperature factors in Table 5 can usefully be compared only with those determined by Blasi *et al.* (1984b) for their two Pikes Peak specimens. By contrast, the shape and orientation of the thermal ellipsoid for the *M* atom can be compared in all four specimens considered above.

Most of the U_{ij} values in Table 5 tend to be slightly higher than the corresponding data for the two Pikes Peak specimens of Blasi *et al.* (1984b). This tendency is more evident with respect to 7813B than 7813A. The *B*eq values in Table 5 behave in a similar way to those of the parent anisotropic data. Apart from the experimental error, the differences found between corresponding values of thermal parameters in these three specimens could be the result of a combination of effects related to small variations in Si,Al distribution and, more probably, in Na substitution, which is slightly higher in the Pellotsalo microcline (Tables 1, 3). The structure refinement of a fully K-exchanged low microcline could clarify the question.

The thermal ellipsoid for the *M* atom is disc-shaped, with two long axes and one short axis (Table 5), as found by Brown & Bailey (1964) and Blasi *et al.* (1984b) in their specimens. The short axis is almost parallel to X^* in all four specimens. The two other axes are symmetrically disposed about *Z* in the specimens of Brown & Bailey (1964) and Blasi *et al.* (1984b), whereas they are close to *Y* and *Z* in the microcline investigated in this paper (Table 5). This discrepancy is only apparent, as the two long axes in the latter specimen are very similar in length (Table 5). In fact, the distribution of atomic vibrations in a disc-shaped ellipsoidal model is ideally described solely by the orientation of the shortest axis. Further refinements of the structure of other specimens of low microcline are desirable to gain more insight into the orientation of the two long axes.

Interatomic distances and angles

Each of the 81 interatomic distances and angles in Table 6 was plotted *versus* the mean *T*1*o*–O distance along with the corresponding data for all refinements of $C\bar{1}$ K-rich feldspar [except the Pontiskalk microcline of Finney & Bailey (1964)]. These 81 diagrams show that all the data in Table 6 fit the trend followed by most of the other specimens very closely. Similar behavior is shown by most of the Brown & Bailey (1964) data. Only about one-quarter of these data shows appreciable perturbations. These are related to the positional co-ordinates, which were mentioned earlier to differ most from those given in Table 5. In fact, the most evident perturbations are in distances O*A*2–O*Bo* and O*Bo*–O*Dm* in the *T*2*o* tetrahedron, O*Bm*–O*Co* in the *T*2*m* tetrahedron, and *T*2*m*–O*Bm* as well as in angles O*A*1–*T*1*m*–O*Cm*, *T*1*m*–O*Cm*–*T*2*o*, and *T*1*m*–O*Dm*–*T*2*o*.

However, the values of the interatomic distances and angles determined by Brown & Bailey (1964) are, on the whole, internally consistent and indicate a degree of Si,Al order somewhat higher than that found in the specimen investigated in the present paper. The mean of the four *T*1*o*–O*A*1, –O*Bo*, –O*Co*, –O*Do* bond lengths, which gives an estimate of the average Al–O distance in fully ordered microcline, is in fact appreciably smaller in our specimen (Table 6) than in that of Brown & Bailey (1964). In addition, the mean of the twelve *T*1*m*–O*A*1, –O*Bm*, –O*Cm*, –O*Dm*, *T*2*o*–O*A*2, –O*Bo*, –O*Cm*, –O*Dm*, *T*2*m*–O*A*2, –O*Bm*, –O*Co*, –O*Do* bond lengths, which gives an estimate of the average Si–O distance in fully ordered microcline, is higher in our specimen (Table 6) than in that of Brown & Bailey (1964).

The structural results presented in Table 6 are very similar to the corresponding data on the Prilep microcline of Strob (1983) and the two Pikes Peak specimens of Blasi *et al.* (1984b). In all four of these specimens, structural data provide much the same response as the metric properties. The Pellotsalo microcline of Brown & Bailey (1964) differs in that its structural data are consistent with a degree of Si,Al ordering somewhat higher than that indicated by its metric properties [#2 (reciprocal data) or #3, Table 3].

Comparison of the data reported in this paper with those on the Prilep specimen of Strob (1983) and the two Pikes Peak feldspars of Blasi *et al.* (1984b) suggests that the metric parameters of Brown & Bailey (1964) [#2 (reciprocal data) or #3, Table 3] properly describe the structural state of their Pellotsalo microcline. Conversely, the deviations in interatomic distances and angles in the Pellotsalo feldspar of Brown & Bailey (1964) from the corresponding data from the other specimens of microcline mentioned above should be considered to be anomalous. In this respect, the new data in Table 6 should be regarded as representative of the two Pellotsalo specimens.

MEAN Al–O AND Si–O DISTANCES

The mean *T*–O distances, <*T*–O>, for the six most ordered specimens of microcline used in structure refinements are listed in Table 7. On the basis of previous findings, the data obtained by film methods for specimens 1 and 2 should be considered to be superseded. The recent data obtained by counter methods from specimens 3, 4, 5 and 6 are in excellent agreement with each other. It is worth mentioning that the slight shortening observed by Blasi *et al.* (1984b, p. 419-420) in their Pikes Peak specimen 7813B for the <*T*1*m*–O> distance with respect to both the <*T*2*o*–O> and <*T*2*m*–O> distances also

TABLE 7. MEAN *T*-O, Al-O, AND Si-O DISTANCES, <Al-O>-<Si-O> DIFFERENCES, AND TETRAHEDRAL SITE-OCCUPANCIES FOR SPECIMENS OF LOW MICROCLINE

#	Feldspar Reference	<*T*1*o*-O>† <*T*1*m*-O>† <*T*2*o*-O>† <*T*2*m*-O>†	<Al-O>†§	<Si-O>†¶	Δ=<Al-O>-<Si-O>†x	t1o†∇	t1m†∇	t2o†∇	t2m†∇
		ångströms	ångströms	ångströms	ångströms	with Δ=0.124 Å with Δ=0.125 Å	with Δ=0.124 Å with Δ=0.125 Å	with Δ=0.124 Å with Δ=0.125 Å	with Δ=0.124 Å with Δ=0.125 Å
1	Pellotsalo Brown & Bailey (1964)	1.7407(24) 1.6140(24) 1.6105(24) 1.6115(24)	1.7407(24)	1.6120(14)	0.1288(28)	1.029(17) 1.023(17)	0.007(17) 0.008(17)	-0.022(17) -0.019(17)	-0.014(17) -0.012(17)
2	Pontiskalk Finney & Bailey (1964)+	1.7347(60) 1.6132(60) 1.6190(60) 1.6092(60)	1.7347(60)	1.6138(35)	0.1209(69)	0.981(42) 0.976(42)	0.002(42) 0.004(42)	0.048(42) 0.050(42)	-0.031(42) -0.028(42)
3	Prilep Strob (1983)≡	1.738 1.613 1.614 1.615	1.738	1.614	0.124	1.000 0.994	-0.008 -0.006	0.000 0.002	0.008 0.010
4	Pikes Peak 7813A Blasi *et al.* (1984b)	1.7372(15) 1.6152(15) 1.6120(15) 1.6142(15)	1.7372(15)	1.6138(9)	0.1234(17)	0.996(10) 0.991(10)	0.013(10) 0.015(10)	-0.014(10) -0.011(10)	0.005(10) 0.007(10)
5	Pikes Peak 7813B Blasi *et al.* (1984b)	1.7385(15) 1.6120(14) 1.6152(15) 1.6135(15)	1.7385(15)	1.6136(8)	0.1249(17)	1.006(10) 1.000(10)	-0.015(10) -0.012(10)	0.012(10) 0.014(10)	-0.003(10) 0.000(10)
6	Pellotsalo This work	1.7377(15) 1.6127(11) 1.6140(14) 1.6137(14)	1.7377(15)	1.6135(8)	0.1242(17)	1.002(10) 0.996(10)	-0.007(9) -0.004(8)	0.004(10) 0.006(10)	0.002(10) 0.004(10)

Estimated standard errors (1σ) are given in parentheses and refer to the last decimal place.

† σ values were obtained from the Law of Propagation of Errors (see Blasi 1977) using everywhere standard errors of individual *T*-O distances and assuming that (a) individual *T*-O distances can be considered as uncorrelated, (b) co-variance terms can be neglected, and (c) Δ coefficients, which are involved only in the calculations of Al contents, can be treated as constants.

§ <Al-O> was assumed to be equal to <*T*1*o*-O>.

¶ <Si-O> was assumed to be equal to the average of the *T*1*m*-O*A*1, -O*Bm*, -O*Cm*, -O*Dm*, *T*2*o*-O*A*2, -O*Bo*, -O*Cm*, -O*Dm*, *T*2*m*-O*A*2, -O*Bm*, -O*Co*, -O*Do* distances.

x Δ values were calculated starting from individual *T*-O distances rather than mean *T*-O distances.

∇ Al contents of *T*1*o*, *T*1*m*, *T*2*o*, and *T*2*m* sites were calculated using the procedure of Kroll & Ribbe (1983, p. 67, equation 5) with the two different Δ values indicated in the relevant column headings. Except for Prilep microcline (Strob 1983, see footnote ≡), the calculations were done starting from individual *T*-O distances rather than mean *T*-O distances and grand mean *T*-O values derived from mean *T*-O data. This procedure was used to reduce truncation and/or rounding errors which could amount to 4 digits in the third decimal place of Al contents.

+ Following two different procedures, Finney & Bailey (1964) estimated the standard error in each of their individual *T*-O distances to be 0.012 or 0.019 Å, respectively. The former value was involved in the present calculations, considering that it was also used by Finney & Bailey (1964, p. 425) for testing the significance of their mean *T*-O distances.

≡ Individual *T*-O distances and standard errors were not available.

occurs in the Pellotsalo feldspar investigated in this paper as well as in the Prilep microcline of Strob (1983) (Table 7). This effect, which no longer seems to be an idiosyncratic feature of low albite alone, should be investigated.

Table 7 also gives the values of the mean Al–O and Si–O distances, <Al–O> and <Si–O>, along with their Δ differences for all six specimens considered. These quantities are of primary importance, since the reference values to be used in the appropriate formulations for converting <*T*–O> distances to Al contents in K-rich feldspars must be chosen from amongst them. Ribbe (1975), Kroll & Ribbe (1983) and Ribbe (1984) found that it is more convenient to enter a Δ difference rather than <Al–O> and <Si–O> distances themselves in the equations used for converting <*T*–O> distances to Al contents. The Δ value behaves in essence as a scale factor. When the Δ value of the feldspar investigated here is used to convert <*T*–O> distances to Al contents in the specimen of Brown & Bailey (1964), the latter will appear to be a hyperordered microcline. Conversely, the Δ value of Brown & Bailey (1964) feldspar will make the microcline of this investigation appear to be slightly disordered.

The formulation proposed by Smith (1974a) for converting <*T*–O> distances to Al contents in all feldspars involves a Δ value of 0.133 Å. This procedure, however, was developed before the new data for specimens 3, 4, 5 and 6 in Table 7 became available. Ribbe (1975) adopted a Δ value of 0.130 Å for all feldspars. Subsequently, Kroll & Ribbe (1983) and Ribbe (1984) proposed a Δ value of 0.125 Å for K-rich feldspar. The latter was obtained by averaging the Δ values in specimens 1, 2, 3, 4 and 5 in Table 7. The present study suggests that in K-rich feldspars, a new reference value for Δ could be taken equal to 0.124 Å, when adopting the average of the Δ data for specimens 3, 4, 5 and 6 in Table 7. On the other hand, a Δ value of 0.125 Å could also be adopted, since it corresponds to that of the Pikes Peak specimen 7813B, which appears to be the most ordered microcline in Table 7. The latter value happens to be the same as that already proposed by Kroll & Ribbe (1983) and Ribbe (1984), owing to the fact that Δ values for the two superseded specimens 1 and 2 in Table 7, *i.e.*, 0.129 and 0.121 Å, respectively, compensate each other in such a way that the relevant mean is exactly equal to 0.125 Å.

For convenience, Table 7 also gives Al contents in the *T* sites calculated in all six specimens of microcline using the formulation of Kroll & Ribbe (1983) with a Δ value of either 0.124 or 0.125 Å. It is to be hoped that the Δ value will be further improved in the near future by new structure refinements of specimens of fully ordered low microcline.

The new data obtained for the Pellotsalo microcline further confirm that the behavior of the <Al–O> and <Si–O> bond lengths differs in K-rich and Na-rich feldspars. In fact, on the basis of the structural data obtained by Starkey & Wainwright (1970), Harlow & Brown (1980) and Wenk & Kroll (1984), samples of Na-rich feldspar show a Δ value of 0.129 Å. In agreement with Kroll & Ribbe (1983) and Ribbe (1984), then, the formulations for converting <*T*–O> distances to Al contents should use different Δ values in K-rich *versus* Na-rich feldspars.

GENETIC CONSIDERATIONS

Although the Pellotsalo maximum microcline has aroused interest from a number of mineralogists and petrologists since the beginning of this century, the interpretation of its genetic conditions is still open to question. In a discussion of his goniometric measurements on some specimens of microcline from Tammela, Finland, and Pellotsalo, Mäkinen (1913, p. 60-61) claimed that partly cross-hatched microcline derives from untwinned microcline or orthoclase. Eskola (1951, p. 40) doubted the assertion of Laves (1950) that cross-hatching is a consequence of inversion from a monoclinic state and reported that the observations by Mäkinen and himself show that the Pellotsalo specimen formed as a triclinic phase and twinned regions developed later on as a result of secondary deformation. Goldsmith & Laves (1954, p. 113-114) had no doubt that the Pellotsalo microcline formed from a pre-existing monoclinic K-rich feldspar. In a discussion of twinning in microcline, Smith (1974b, p. 388) stated that the origin of untwinned microcline or of microcline with patches of twinning is equivocal. More recently, the intricacies of twinning in microcline have been thoroughly illustrated by Eggleton & Buseck (1980), Brown (1983), Ribbe (1983), Parsons & Brown (1984) and McLaren (1984), among others.

Close examination of the diffraction spots in single-crystal X-ray precession and oscillation photographs obtained in the present investigation shows no evidence of monoclinic ancestry in the K-rich phase of the Pellotsalo feldspar. However, the shape and position of the diffraction spots from the coexisting Na-rich phase may be interpreted in favor of an incipient M-twinning, which would indicate that exsolution took place in a monoclinic environment.

The texture and composition of the perthitic intergrowth from the pegmatite at Pellotsalo provide significant additional data to unravelling the specimen's genetic conditions. In thin sections, the individual components of the perthite show mutual subregular orientations characteristic of exsolution rather than replacement. An exsolution mechanism is also propounded by Mason (1982, p. 103). The composition of the K-rich phase (Tables 1, 3; see also Smith 1974b, Table 19.5, and Mason 1982, Table II) and that of the Na- rich lamellae (Table 1; see also Smith 1974b, Table 19.5, and Mason 1982, Table II) is very pure. No appreciable variation in the Or content of the K-rich component was found either in this investigation or by Smith (1974b, Table 19.5), whereas the Na-rich lamellae show a small increase in Or by 0.3 mol.% and An by 0.2 mol.% in passing from the core to the rim (Smith 1974b, Table 19.5). The absence of compositional disturbances and the uniform cathodoluminescence in each of the two components in the Pellotsalo microperthite would seem to rule out any replacement process. Assuming that the Pellotsalo microperthite formed by exsolution, the high Na content of its bulk composition ($Or_{72}Ab_{27}An_1$ mol.%: Goldsmith & Laves 1961) is of key importance in suggesting primary growth in the monoclinic field in each of the phase diagrams for alkali feldspars proposed by Smith (1974a, Fig. S-1), Martin (1974, Fig. 2), Martin & Bonin (1976, Figs. 3, 4) and Brown & Parsons (1984, Fig. 9), among others. The moderate enrichment in Rb and the low concentration of Ba in the K-rich phase of the Pellotsalo microperthite (Table 1; see also Mason 1982, Table II and Fig. 6) indicate that primary growth took place in a later stage of crystallization at a relatively low temperature. It is therefore probable that the Pellotsalo microperthite formed at a temperature just above that of the $C2/m \rightarrow C\bar{1}$ inversion, which is assumed by Parsons & Brown (1984) to occur in the range 500–400°C at low pressure.

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