

Crystal structure of an authigenic maximum microcline

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With 5 figures

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Auszug

Die Struktur eines authigenen Mikroklins aus dem Pontiskalk, Schweiz, wurde auf Grund von 797 beobachteten und 207 nicht-beobachteten Reflexen verfeinert. Die Ordnung der tetraëdrisch umgebenen Si,Al-Atome ist nahezu vollständig; die Struktur unterscheidet sich nur unbedeutend von derjenigen eines Maximum-Mikroklins magmatischer Herkunft. Es ist anzunehmen, daß der Kristall sehr langsam bei niedriger Temperatur im Stabilitätsbereich der vollkommen geordneten Phase gewachsen ist.

Abstract

The structure of an authigenic maximum microcline from the Pontiskalk limestone, Switzerland, has been refined to an R value of 8.5% by a full-matrix least-squares program using 797 observed and 207 unobserved reflections. The ordering of tetrahedral Si,Al atoms is nearly complete and there is no significant structural difference from an igneous maximum microcline. The crystal is considered to have grown very slowly at a low temperature within the stability field of the fully ordered phase.

Introduction

Small euhedral crystals of potassic or sodic feldspars are not uncommon in the insoluble residues of limestones, or in sandstones and shales. In extreme cases the crystals may make up to 50% of the total rock volume. Optical examination shows that some of the euhedral feldspars are homogeneous units and that others consist of secondary overgrowths on cores of irregular detrital grains or on carbonaceous matter. These authigenic feldspars are believed to have grown very slowly during the diagenetic history of the sediment,

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perhaps beginning shortly after compaction and continuing, for some specimens, through later stage dolomitization and recrystallization. BASKIN² has summarized many of the occurrences and theories of origin.

The potassic authigenic feldspars may be either monoclinic or triclinic. The triclinic specimens exhibit triclinic morphology and appear to represent equilibrium development of the ordered state during growth. Igneous microclines, in contrast, normally exhibit monoclinic morphology. They have formed initially in the disordered state and have reached the ordered triclinic state by solid-state diffusion.

The degree of tetrahedral Si, Al order in several potassic feldspars has been well documented by COLE, SÖRUM and KENNARD³ and RIBBE⁴ for high sanidine, by JONES and TAYLOR⁵ for orthoclase, by BAILEY and TAYLOR⁶ for intermediate microcline, and by BROWN and BAILEY⁷ for an igneous maximum microcline. In all of these specimens, except the heat-treated sanidine, crystallization took place at the relatively high temperatures characteristic of igneous rocks. It is probable that all of these specimens were considerably disordered with respect to Si, Al distribution at crystallization and that they achieved either a partially or completely ordered distribution by following an ordering path during cooling such as those outlined by LAVES⁸, LAVES and GOLDSMITH⁹, SMITH and MACKENZIE¹⁰, or BROWN¹¹. It is of interest to compare these feldspar structures with one believed to have grown

² Y. BASKIN, A study of authigenic feldspars. *J. Geology* **64** (1956) 132–155.

³ W. F. COLE, H. SÖRUM and O. KENNARD, The crystal structures of orthoclase and sanidinized orthoclase. *Acta Crystallogr.* **2** (1949) 280–287.

⁴ P. H. RIBBE, A refinement of the crystal structure of sanidinized orthoclase. *Acta Crystallogr.* **16** (1963) 426–427.

⁵ J. B. JONES and W. H. TAYLOR, The structure of orthoclase. *Acta Crystallogr.* **14** (1961) 443–456.

⁶ S. W. BAILEY and W. H. TAYLOR, The structure of a triclinic potassium feldspar. *Acta Crystallogr.* **8** (1955) 621–632.

⁷ B. E. BROWN and S. W. BAILEY, The structure of maximum microcline. *Acta Crystallogr.* (in press).

⁸ F. LAVES, Al/Si-Verteilungen, Phasen-Transformationen und Namen der Alkalifeldspäte. *Z. Kristallogr.* **113** (1960) 265–296.

⁹ F. LAVES and J. R. GOLDSMITH, Polymorphism, order, disorder, diffusion and confusion in the feldspars. *Inst. "Lucas Mallada" Cursos y Conf.* **8** (1961) 71–80.

¹⁰ J. V. SMITH and W. S. MACKENZIE, Atomic, chemical and physical factors that control the stability of alkali feldspars. *Inst. "Lucas Mallada" Cursos y Conf.* **8** (1961) 39–52.

¹¹ B. E. BROWN, Aluminum distribution in an igneous maximum microcline and the sanidine microcline series. *Norsk Geol. Tidsskr.* **42** (2) (1962) 25–36.

directly in the ordered state at a very low temperature. The present investigation was undertaken to compare the structure of an authigenic maximum microcline with that of the igneous maximum microcline studied by BROWN and BAILEY⁷ in order to provide additional data on the stability relations of microcline.

Material

PERRENOUD¹² and BASKIN² have previously described well formed microcline crystals in the Pontiskalk formation, a compact dolomitic limestone of Triassic age in the Swiss Alps. Some of these crystals were concentrated and supplied to us by Prof. F. LAVES.

The crystals are triclinic units, 0.1 to 1.0 mm in size, often with sector-like fourling twins. These unique twins have never been observed in non-authigenic microclines and have been explained by BASKIN² as resulting from a combination of the albite and pericline twin laws. Some crystals have visible cores of rounded feldspar grains, usually containing a large number of dark, extremely fine inclusions. Most of the grains have a mottled appearance under the polarizing microscope, and have poor extinctions except on (001). Zoning and crystal aggregates are common.

Although good single crystals are very rare, it was possible to cut a suitable piece having good extinction from the outer edge of one of the sectors of a large crystal, taking care to avoid any of the core material. The crystal obtained measures $0.11 \times 0.13 \times 0.18$ mm. All of the experimental data were obtained from this one crystal. The spot shapes are quite good, but have a slight streaking due to mosaic spread that becomes more pronounced for higher levels.

BASKIN² cites a spectrographic analysis of purified material that showed only 0.2% Na₂O, not all of which may be in the microcline. The extreme purity is verified by the $d(\bar{2}01)$ and $d(400)$ values of 4.218 Å and 1.926 Å, respectively. In fact, GOLDSMITH and LAVES¹³ have used Pontiskalk crystals as their purest microcline reference material in constructing spacing-composition curves. The maximum obliquity of the crystal used is verified by its Δ value of 0.97 and its γ^* angle of $92^\circ 13'$.

¹² J.-P. PERRENOUD, Etude du feldspath potassique contenu dans le "Pontiskalk" (Trias, Valais). Schweiz. Mineral. Petrogr. Mitt. **32** (1952) 179–184.

¹³ J. R. GOLDSMITH and F. LAVES, The sodium content of microclines and the microcline-albite series. Inst. "Lucas Mallada" Cursos y Conf. **8** (1961) 81–96.

Experimental

Accurate cell dimensions were obtained by the θ method of WEISZ, COCHRAN and COLE¹⁴. Optical measurements were made using the spindle mount of WILCOX¹⁵ on a five-axis universal stage. The unit-cell parameters and optical measurements are listed in Table 1.

Table 1. Unit-cell dimensions and optical properties for the Pontiskalk microcline

	$C\bar{1}$	$P\bar{1}$			
α^*	.12981 Å ⁻¹	.14842 Å ⁻¹	N	1.5178	
b^*	.07721	.15362		β	1.5218
c^*	.15405	.15405		γ	1.5243
α^*	90° 28'	111° 46'	$2V_{\text{meas.}}$	77.0°	
β^*	64° 04'	67° 40'	$2V_{\text{calc.}}$	76.5°	
γ^*	92° 13'	118° 32'	"b" - α	.0065	
a	8.5726 Å	7.9205 Å	Extinction on (001)	16.5°	
b	12.9618	7.6219			
c	7.2188	7.2188			
α	90° 34'	76° 33'			
β	115° 55'	104° 23'			
γ	87° 45'	66° 52'			
V	721.3 Å ³	360.5 Å ³			

A total of 797 observed reflections were obtained by Weissenberg techniques using MoK α radiation and triple film packs interleaved with tin foil. Data were collected for the zero levels about the [110], [$\bar{1}\bar{1}0$], and [001] zones and for the first level on [001]. Exposure times ranged from 5 to 100 hours. Intensities were measured visually by comparing them with known intensities on a triple film-pack scale. A different set of scales was prepared for each orientation to allow for changes in spot size and shape. Corrections were applied for the Lorentz-polarization factors and for increasing separation of the α_1 - α_2 doublet, but no absorption correction was attempted.

Absolute scaling of structure amplitudes was accomplished by comparing them with the Pellotsalo maximum-microcline data of BROWN and BAILEY⁷. The space group was assumed to be $C\bar{1}$, as for the Pellotsalo material, because of the close correspondence of structure amplitudes of the two microclines and the absence of any reflections or streaks for $h+k=2n+1$.

¹⁴ O. WEISZ, W. COCHRAN and W. F. COLE, The accurate determination of cell dimensions from single-crystal x-ray photographs. *Acta Crystallogr.* **1** (1948) 83-88.

¹⁵ R. E. WILCOX, Universal stage accessory for direct determination of the three principal indices of refraction. *Amer. Mineral.* **44** (1959) 1064-1067.

Refinement of the structure

The structure was refined on the basis of a primitive cell for which the zones $[110]$, $[1\bar{1}0]$ and $[001]$ of the centered cell were used as X , Y and Z respectively. A full-matrix least-squares program written for the IBM 704 by A. C. LARSON and D. T. CROMER at the Los Alamos Scientific Laboratory was used in the early stages of the refinement at Los Alamos. The program was modified for use on a CDC 1604 computer, on which the refinement was completed at the University of Wisconsin.

Scattering factor curves from BERGHUIS *et al.*¹⁶ were used for K, Si and O and from PARRY¹⁷ for Al. Si, Al and O were treated as half-ionized atoms and appropriate curves were derived by interpolation. No dispersion corrections were applied and no assumption as to tetrahedral ordering was made at the start. The scattering-factor curves approximate as closely as possible those used for the intermediate microcline of BAILEY and TAYLOR⁶ and for the Pellotsalo maximum microcline of BROWN and BAILEY⁷ in order to facilitate comparison with these structures.

In the first stage of the refinement 315 observed $h0l$ and $0kl$ reflections (primitive cell) were used, with unit weighting and isotropic temperature factors. The atomic positions obtained for the Pellotsalo maximum microcline at the end of its first stage of refinement were used as the starting parameters. Eight least-squares cycles were run, at which point the parameter shifts were insignificant and the R factor had decreased from 12.2 to 10.1%. For the second refinement stage all 797 observed reflections were used in six least-squares cycles with isotropic temperature factors and in four cycles with anisotropic temperature factors for potassium. Reflections having $F_o > 80$ and < 10 were weighted as 0.5. Because temperature factors and bond-length calculations at the end of the first refinement stage indicated nearly complete Si, Al order, the scattering factor of Al was used for $T_1(0)$ and of Si for the other three tetrahedral sites. After all variable parameters had converged the R factor had decreased to 9.4%. As a last refinement step the 207 unobserved reflections were added to the data and were given intensities of one-half the limit of observability. Three

¹⁶ J. BERGHUIS, I. M. HAANAPPEL, M. POTTERS, B. O. LOOFSTRA, C. H. MAC GILLAVRY and A. L. VEENENDAAL, New calculations of atomic scattering factors. *Acta Crystallogr.* 8 (1955) 478–483.

¹⁷ G. S. PARRY, A study of the atomic scattering factor for aluminum. *Acta Crystallogr.* 8 (1955) 593–594.

Table 2. *Final positional and thermal parameters for the Pontiskalk microcline*

Atom*	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i>	σ_m
K	.2831	— .0067	.1360	1.35**	.0006
T ₁ (0)	.0096	.1880	.2179	.60	.0007
T ₁ (<i>m</i>)	.0098	.8191	.2327	.61	.0006
T ₂ (0)	.7117	.1200	.3400	.56	.0006
T ₂ (<i>m</i>)	.7067	.8858	.3495	.54	.0006
O _A (1)	.0007	.1448	— .0179	1.11	.0016
O _A (2)	.6361	.0053	.2862	.58	.0015
O _B (0)	.8218	.1476	.2200	1.14	.0018
O _B (<i>m</i>)	.8307	.8568	.2435	1.42	.0018
O _C (0)	.0347	.3188	.2564	.67	.0015
O _C (<i>m</i>)	.0382	.6955	.2646	.74	.0016
O _D (0)	.1900	.1228	.4055	1.14	.0017
O _D (<i>m</i>)	.1754	.8745	.4091	1.31	.0017

* Prototype atoms with full symbols (0000) or (*m*000).

** Anisotropic temperature factors for K given in Table 7.

least-squares cycles were run utilizing anisotropic temperature factors for potassium and the same weighting scheme as in the previous cycles. The final weighted *R* factor was 8.5%. The final positional and thermal parameters, after conversion to the centered cell, are listed in Table 2. Observed and calculated structure factors are given in Table 3. Bond lengths and angles calculated from these parameters are listed in Table 4.

Accuracy of results

Correlation coefficients were calculated after the last least-squares cycle. Of the 1512 possible nondiagonal coefficients of the half-matrix, only 95 had values greater than 0.10, 14 greater than 0.30, and none over 0.40. Interaction between positional, thermal and scale parameters, therefore, is considered negligible.

The standard deviations of positional parameters were calculated from the expression

$$\sigma_i^2 = \frac{\Sigma w (F_o - F_c)^2}{m - n} \cdot D_{ii} \quad (1)$$

where *w* = weight, *m* = number of observations, *n* = number of variables, and *D_{ii}* = diagonal term of the inverse matrix (variance). Because the data collection does not represent a spherical distribution in reciprocal space and because the three axes are not of equal lengths,

Table 3. Observed and calculated structure factors for the Pontiskalk microcline
h, k, l refer to the primitive cell and *h₁, k₁, l₁* refer to the centered cell

<i>h k l</i>	<i>F_o</i>	<i>F_c</i>	<i>h₁ k₁ l₁</i>	<i>h k l</i>	<i>F_o</i>	<i>F_c</i>	<i>h₁ k₁ l₁</i>	<i>h k l</i>	<i>F_o</i>	<i>F_c</i>	<i>h₁ k₁ l₁</i>
1 11 0	9	-10	12 10 0	4 1 0	35	-36	5 3 0	7 4 0	29	29	3 11 0
2 11 0	8	-3	13 9 0	5 1 0	23	-24	6 4 0	8 4 0	0	1	4 12 0
1 10 0	0	2	11 9 0	7 1 0	12	13	8 6 0	9 4 0	5	1	5 13 0
2 10 0	14	-17	12 8 0	8 1 0	22	-24	9 7 0	10 4 0	0	-3	6 14 0
6 10 0	7	0	16 4 0	9 1 0	6	6	10 8 0	11 4 0	10	8	7 15 0
1 9 0	9	7	10 8 0	10 1 0	7	7	11 9 0	12 4 0	0	3	8 16 0
2 9 0	11	7	11 7 0	2 0 0	75	-75	2 2 0	0 5 0	21	20	9 17 0
3 9 0	0	4	12 6 0	3 0 0	13	9	3 3 0	1 5 0	25	27	10 18 0
5 9 0	0	0	14 4 0	4 0 0	11	-11	4 4 0	2 5 0	14	13	11 19 0
1 8 0	18	-16	9 7 0	5 0 0	23	23	5 5 0	3 5 0	80	-84	12 20 0
2 8 0	8	5	10 6 0	6 0 0	21	22	6 6 0	4 5 0	36	-36	13 21 0
3 8 0	12	11	11 5 0	7 0 0	16	17	7 7 0	5 5 0	37	40	14 22 0
5 8 0	14	-12	13 3 0	8 0 0	16	-16	8 8 0	6 5 0	8	6	15 23 0
1 7 0	17	17	8 2 0	9 0 0	27	-26	9 9 0	7 5 0	17	13	16 24 0
2 7 0	20	17	9 1 0	10 0 0	0	0	10 10 0	8 5 0	17	-15	17 25 0
3 7 0	12	-13	10 0 0	11 0 0	14	8	11 11 0	9 5 0	15	-14	18 26 0
4 7 0	12	-12	11 0 0	12 0 0	0	5	12 12 0	10 5 0	0	1	19 27 0
5 7 0	14	-14	12 0 0	13 0 0	0	-7	13 13 0	11 5 0	0	1	20 28 0
6 7 0	0	3	13 0 0	2 1 0	58	-54	1 3 0	12 5 0	15	15	21 29 0
7 7 0	13	11	14 0 0	3 1 0	20	17	2 4 0	0 6 0	26	26	22 30 0
1 6 0	8	5	7 0 0	4 1 0	33	29	3 5 0	1 6 0	9	-8	23 31 0
2 6 0	17	16	8 0 0	5 1 0	31	29	4 6 0	2 6 0	22	-23	24 32 0
3 6 0	14	-15	9 0 0	6 1 0	11	-8	5 7 0	3 6 0	22	22	25 33 0
4 6 0	0	0	10 0 0	7 1 0	11	-12	6 8 0	4 6 0	0	4	26 34 0
5 6 0	21	22	11 0 0	8 1 0	13	12	7 9 0	5 6 0	0	-3	27 35 0
6 6 0	9	-8	12 0 0	9 1 0	9	7	8 10 0	6 6 0	10	-8	28 36 0
7 6 0	0	3	13 1 0	10 1 0	13	14	9 11 0	7 6 0	6	-4	29 37 0
1 5 0	22	-20	6 0 0	11 1 0	0	-7	10 12 0	8 6 0	18	-16	30 38 0
2 5 0	25	-26	7 0 0	12 1 0	9	-5	11 13 0	9 6 0	5	0	31 39 0
3 5 0	13	-13	8 0 0	13 1 0	8	4	12 14 0	10 6 0	21	23	32 40 0
4 5 0	15	-16	9 1 0	0 2 0	75	-75	2 2 0	11 6 0	9	-8	33 41 0
5 5 0	25	26	10 0 0	1 2 0	35	-36	3 3 0	12 6 0	11	-11	34 42 0
6 5 0	18	20	11 1 0	2 2 0	36	-39	4 4 0	0 7 0	12	12	35 43 0
7 5 0	11	-7	12 2 0	3 2 0	8	2	1 5 0	1 7 0	12	-12	36 44 0
8 5 0	11	-12	13 3 0	4 2 0	19	17	2 6 0	2 7 0	32	-37	37 45 0
1 4 0	38	-35	5 0 0	5 2 0	0	1	3 7 0	3 7 0	20	19	38 46 0
2 4 0	26	-23	6 0 0	6 2 0	9	-4	4 8 0	4 7 0	28	29	39 47 0
3 4 0	37	37	7 1 0	7 2 0	33	-35	5 9 0	5 7 0	19	17	40 48 0
4 4 0	0	1	8 0 0	8 2 0	9	-9	6 10 0	6 7 0	8	-8	41 49 0
5 4 0	15	-14	9 1 0	9 2 0	9	9	7 11 0	7 7 0	16	-12	42 50 0
6 4 0	5	-5	10 2 0	10 2 0	14	15	8 12 0	8 7 0	7	8	43 51 0
7 4 0	15	-15	11 3 0	11 2 0	0	-4	9 13 0	9 7 0	7	-9	44 52 0
8 4 0	7	-1	12 4 0	12 2 0	7	-8	10 14 0	10 7 0	16	15	45 53 0
1 3 0	24	-23	4 0 0	13 2 0	13	12	11 15 0	11 7 0	9	9	46 54 0
2 3 0	12	-9	5 1 0	0 3 0	18	13	12 16 0	12 7 0	12	-12	47 55 0
3 3 0	46	46	6 0 0	1 3 0	25	22	13 17 0	0 8 0	28	-29	48 56 0
4 3 0	33	35	7 1 0	2 3 0	7	-4	14 18 0	1 8 0	15	12	49 57 0
5 3 0	7	-4	8 2 0	3 3 0	76	82	0 6 0	2 8 0	10	10	50 58 0
6 3 0	13	-11	9 3 0	4 3 0	19	17	1 7 0	3 8 0	0	0	51 59 0
7 3 0	15	-16	10 4 0	5 3 0	94	-91	2 8 0	4 8 0	0	-3	52 60 0
8 3 0	12	13	11 5 0	6 3 0	8	7	3 9 0	5 8 0	13	-11	53 61 0
1 2 0	31	32	3 1 0	7 3 0	27	27	4 10 0	6 8 0	16	-15	54 62 0
2 2 0	64	67	4 0 0	8 3 0	9	7	5 11 0	7 8 0	10	-9	55 63 0
3 2 0	8	6	5 1 0	9 3 0	0	-2	6 12 0	8 8 0	41	40	56 64 0
4 2 0	25	-24	6 2 0	10 3 0	20	-19	7 13 0	9 8 0	9	8	57 65 0
5 2 0	31	-32	7 3 0	11 3 0	0	0	8 14 0	10 8 0	24	-25	58 66 0
6 2 0	15	16	8 4 0	12 3 0	7	-6	9 15 0	12 8 0	7	-4	59 67 0
7 2 0	18	20	9 5 0	0 4 0	16	-15	10 16 0	13 8 0	13	12	60 68 0
8 2 0	0	5	10 6 0	1 4 0	27	26	11 17 0	0 9 0	23	-22	61 69 0
9 2 0	13	14	11 7 0	2 4 0	30	29	12 18 0	1 9 0	0	2	62 70 0
10 2 0	12	-11	12 8 0	3 4 0	6	-6	13 19 0	2 9 0	14	14	63 71 0
1 1 0	24	-22	2 0 0	4 4 0	34	36	0 8 0	3 9 0	0	-1	64 72 0
2 1 0	32	31	3 1 0	5 4 0	16	-13	1 9 0	4 9 0	0	4	65 73 0
3 1 0	20	-21	4 2 0	6 4 0	11	-10	2 10 0	5 9 0	21	-21	66 74 0

Table 3 (Continued)

h	k	l	F_o	F_c	h_1	k_1	l_1	h	k	l	F_o	F_c	h_1	k_1	l_1	h	k	l	F_o	F_c	h_1	k_1	l_1
4	1	1	33	-35	5	3	1	8	3	1	21	23	11	5	1	1	6	1	24	25	7	5	1
5	1	1	27	27	6	4	1	7	3	1	6	-4	10	4	1	0	6	1	7	-7	6	6	1
6	1	1	16	15	7	5	1	6	3	1	33	-35	9	3	1	1	6	1	12	9	5	7	1
7	1	1	16	-17	8	6	1	5	3	1	8	-8	8	2	1	2	6	1	17	-16	4	8	1
13	0	1	13	-14	13	13	1	4	3	1	0	-2	7	1	1	3	6	1	0	0	3	9	1
12	0	1	0	-1	12	12	1	3	3	1	26	28	6	0	1	4	6	1	7	8	2	10	1
11	0	1	16	16	11	11	1	2	3	1	10	10	5	1	1	5	6	1	9	7	1	11	1
10	0	1	0	2	10	10	1	1	3	1	10	-7	4	2	1	6	6	1	28	29	0	12	1
9	0	1	0	-1	9	9	1	0	3	1	32	-31	3	3	1	7	6	1	13	-10	1	13	1
8	0	1	15	-16	8	8	1	1	3	1	57	-65	2	4	1	8	6	1	0	1	2	14	1
7	0	1	0	-3	7	7	1	2	3	1	24	26	1	5	1	9	6	1	10	11	3	15	1
6	0	1	0	-3	6	6	1	3	3	1	26	26	0	6	1	10	6	1	0	0	4	16	1
5	0	1	8	8	5	5	1	4	3	1	17	15	1	7	1	11	6	1	0	1	5	17	1
4	0	1	40	40	4	4	1	5	3	1	18	16	2	8	1	12	6	1	0	-1	6	18	1
3	0	1	42	-42	3	3	1	6	3	1	7	-7	3	9	1	4	7	1	0	3	11	3	1
2	0	1	30	-31	2	2	1	7	3	1	3	0	4	10	1	3	7	1	0	-1	10	4	1
1	0	1	37	32	1	1	1	8	3	1	19	-16	5	11	1	2	7	1	26	-27	9	5	1
2	0	1	14	-13	2	2	1	9	3	1	17	15	6	12	1	1	7	1	16	18	8	6	1
3	0	1	18	17	3	3	1	10	3	1	21	22	7	13	1	0	7	1	7	7	7	7	1
4	0	1	10	-10	4	4	1	12	3	1	0	1	9	15	1	1	7	1	12	-12	6	8	1
5	0	1	31	-30	5	5	1	8	4	1	0	-7	12	4	1	2	7	1	8	-6	5	9	1
6	0	1	0	1	6	6	1	7	4	1	8	9	11	3	1	3	7	1	9	-8	4	10	1
7	0	1	11	-10	7	7	1	6	4	1	13	-12	10	2	1	4	7	1	6	-7	3	11	1
8	0	1	26	26	8	8	1	5	4	1	0	4	9	1	1	5	7	1	32	-32	2	12	1
9	0	1	0	2	9	9	1	4	4	1	22	24	8	0	1	6	7	1	0	5	1	13	1
10	0	1	0	-5	10	10	1	3	4	1	0	2	7	1	1	7	7	1	28	25	0	14	1
11	0	1	0	-4	11	11	1	2	4	1	29	-31	6	2	1	8	7	1	5	2	1	15	1
12	0	1	0	-7	12	12	1	1	4	1	17	-15	5	3	1	9	7	1	16	-16	2	16	1
9	1	1	13	-14	10	8	1	0	4	1	37	37	4	4	1	10	7	1	12	-11	3	17	1
8	1	1	6	2	9	7	1	1	4	1	22	-23	3	5	1	11	7	1	15	13	4	18	1
7	1	1	27	28	8	6	1	2	4	1	24	-25	2	6	1	12	7	1	0	-3	5	19	1
6	1	1	24	23	7	5	1	3	4	1	9	-7	1	7	1	4	8	1	12	-11	12	4	1
5	1	1	42	-43	6	4	1	4	4	1	9	-6	0	8	1	3	8	1	20	22	11	5	1
4	1	1	9	-6	5	3	1	5	4	1	8	7	1	9	1	2	8	1	17	19	10	6	1
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3	1	1	52	-52	2	4	1	9	4	1	28	-26	5	13	1	2	8	1	0	2	6	10	1
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5	1	1	10	-9	4	6	1	11	4	1	9	8	7	15	1	4	8	1	32	30	4	12	1
6	1	1	14	-14	5	7	1	12	4	1	0	-3	8	16	1	5	8	1	4	0	3	13	1
7	1	1	0	2	6	8	1	8	5	1	15	-17	13	3	1	6	8	1	22	-20	2	14	1
8	1	1	6	1	7	9	1	7	5	1	11	-10	12	2	1	7	8	1	0	0	1	15	1
9	1	1	11	-13	8	10	1	6	5	1	0	3	11	1	1	8	8	1	20	-14	0	16	1
10	1	1	11	-11	9	11	1	5	5	1	17	19	10	0	1	9	8	1	0	3	1	17	1
12	1	1	0	3	11	13	1	4	5	1	10	10	9	1	1	10	8	1	0	-1	2	18	1
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7	2	1	16	-17	9	5	1	2	5	1	18	19	7	3	1	3	9	1	8	2	12	6	1
6	2	1	19	19	8	4	1	1	5	1	36	-40	6	4	1	1	9	1	12	-11	10	8	1
5	2	1	13	13	7	3	1	0	5	1	5	-5	5	5	1	0	9	1	0	2	9	9	1
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3	2	1	14	13	5	1	1	2	5	1	11	10	3	7	1	2	9	1	12	11	7	11	1
2	2	1	37	33	4	0	1	3	5	1	22	23	2	8	1	3	9	1	16	-15	6	12	1
1	2	1	16	14	3	1	1	4	5	1	10	-10	1	9	1	4	9	1	0	-3	5	13	1
0	2	1	14	-14	2	2	1	5	5	1	10	-10	0	10	1	5	9	1	27	26	4	14	1
1	2	1	21	23	1	3	1	6	5	1	12	-10	1	11	1	7	9	1	10	8	2	16	1
2	2	1	45	47	0	4	1	7	5	1	20	-19	2	12	1	8	9	1	0	-4	1	17	1
3	2	1	21	-23	1	5	1	8	5	1	23	23	3	13	1	9	9	1	0	-1	0	18	1
4	2	1	17	-17	2	6	1	9	5	1	12	12	4	14	1	10	9	1	4	5	1	19	1
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7	2	1	0	2	5	9	1	12	5	1	9	-8	7	17	1	1	10	1	10	-12	11	9	1
8	2	1	14	-15	6	10	1	6	6	1	16	16	12	0	1	0	10	1	0	1	10	10	1
9	2	1	0	4	7	11	1	4	6	1	12	-13	10	1	1	1	10	1	10	-11	9	11	1
10	2	1	22	-20	8	12	1	3	6	1	27	-28	9	3	1	2	10	1	7	2	8	12	1
12	2	1	13	12	10	14	1	2	6	1	7	7	8	4	1	3	10	1	19	18	7	13	1

Table 3 (Continued)

h	k	l	F _o	F _c	h ₁	k ₁	l ₁	h	k	l	F _o	F _c	h ₁	k ₁	l ₁	h	k	l	F _o	F _c	h ₁	k ₁	l ₁
4	10	1	19	-18	6	14	1	0	10	2	15	-15	10	10	2	4	0	4	14	-15	4	4	4
5	10	1	0	-6	5	15	1	0	11	2	0	-5	11	11	2	5	0	4	0	4	5	5	4
8	10	1	11	10	2	18	1	0	11	3	0	-5	11	11	3	6	0	4	20	22	6	6	4
9	10	1	0	-3	1	19	1	0	9	3	0	-4	9	9	3	7	0	4	10	-11	7	7	4
10	10	1	13	12	0	20	1	0	8	3	6	-6	8	8	3	8	0	4	0	4	8	8	4
12	10	1	14	-12	2	22	1	0	7	3	6	-1	7	7	3	0	1	4	6	-7	1	1	4
0	11	1	5	4	11	11	1	0	6	3	7	7	6	6	3	0	2	4	8	9	2	2	4
1	11	1	10	9	10	12	1	0	5	3	13	13	5	5	3	0	3	4	17	-18	3	3	4
2	11	1	15	-16	9	13	1	0	4	3	48	-49	4	4	3	0	4	4	0	-3	4	4	4
3	11	1	6	-5	8	14	1	0	3	3	9	-9	3	3	3	0	5	4	7	7	5	5	4
4	11	1	9	8	7	15	1	0	2	3	26	26	2	2	3	0	6	4	19	19	6	6	4
5	11	1	0	-3	6	16	1	0	1	3	41	-37	1	1	3	0	7	4	8	-10	7	7	4
8	11	1	0	0	5	19	1	12	0	3	17	12	12	12	3	0	8	4	6	-6	8	8	4
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10	11	1	0	1	1	21	1	10	0	3	10	-12	10	10	3	0	8	5	0	-7	8	8	5
1	12	1	14	14	11	13	1	9	0	3	0	1	9	9	3	0	7	5	0	-4	7	7	5
2	12	1	0	4	10	14	1	8	0	3	17	20	8	8	3	0	6	5	6	-5	6	6	5
3	12	1	12	-8	9	15	1	7	0	3	16	18	7	7	3	0	5	5	12	13	5	5	5
8	12	1	13	13	4	20	1	6	0	3	12	-11	6	6	3	0	4	5	27	30	4	4	5
10	12	1	13	-13	2	22	1	5	0	3	24	29	5	5	3	0	3	5	28	-31	3	3	5
1	13	1	12	-12	12	14	1	4	0	3	0	-4	4	4	3	0	2	5	17	-17	2	2	5
5	14	1	4	-1	9	19	1	3	0	3	28	-28	3	3	3	0	1	5	12	13	1	1	5
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0	9	2	13	15	9	9	2	1	0	3	27	28	1	1	3	5	0	5	9	-10	9	9	5
0	8	2	0	-1	8	8	2	0	0	3	19	16	0	0	3	8	0	5	21	-22	8	8	5
0	7	2	0	6	7	7	2	1	0	3	43	-43	1	1	3	7	0	5	0	-5	7	7	5
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12	0	2	0	1	12	12	2	9	0	3	0	-7	9	9	3	1	0	5	25	23	1	1	5
11	0	2	16	-13	11	11	2	0	1	3	34	30	1	1	3	2	0	5	0	5	2	2	5
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8	0	2	28	30	8	8	2	0	4	3	10	10	4	4	3	5	0	5	18	15	5	5	5
7	0	2	10	-8	7	7	2	0	5	3	35	36	5	5	3	6	0	5	11	-6	6	6	5
6	0	2	23	-24	6	6	2	0	6	3	21	-25	6	6	3	7	0	5	0	-1	7	7	5
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4	0	2	27	-26	4	4	2	0	8	3	19	20	8	8	3	0	1	5	32	32	1	1	5
3	0	2	22	-20	3	3	2	0	9	3	5	-2	9	9	3	0	2	5	4	4	2	2	5
2	0	2	27	26	2	2	2	0	10	3	0	-7	10	10	3	0	3	5	5	-3	3	3	5
1	0	2	56	54	1	1	2	0	8	4	9	8	8	8	4	0	4	5	49	-45	4	4	5
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3	0	2	12	11	3	3	2	0	4	4	8	-9	4	4	4	0	8	5	17	-20	8	8	5
4	0	2	25	26	4	4	2	0	3	4	0	-1	3	3	4	0	9	5	15	-13	9	9	5
5	0	2	23	-23	5	5	2	0	2	4	15	-15	2	2	4	0	13	5	7	9	13	13	5
6	0	2	14	-14	6	6	2	0	1	4	30	31	1	1	4	0	14	5	7	-12	14	14	5
7	0	2	13	12	7	7	2	10	0	4	0	-2	10	10	4	0	8	6	7	8	8	8	6
8	0	2	10	-6	8	8	2	9	0	4	16	18	9	9	4	0	7	6	13	14	7	7	6
9	0	2	16	14	9	9	2	8	0	4	11	-10	8	8	4	0	6	6	12	-11	6	6	6
10	0	2	12	8	10	10	2	7	0	4	17	-21	7	7	4	0	5	6	0	4	5	5	6
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0	3	2	21	-18	3	3	2	3	0	4	11	-13	3	3	4	0	1	6	7	7	1	1	6
0	4	2	22	-21	4	4	2	2	0	4	9	-7	2	2	4	10	0	6	11	8	10	10	6
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0	7	2	5	3	7	7	2	1	0	4	50	48	1	1	4	7	0	6	15	19	7	7	6
0	8	2	34	37	8	8	2	2	0	4	11	-10	2	2	4	6	0	6	0	2	6	6	6
0	9	2	0	-3	9	9	2	3	0	4	12	-10	3	3	4	5	0	6	9	6	5	5	6

Table 3 (Continued)

h	k	l	F _o	F _c	h ₁	k ₁	l ₁	h	k	l	F _o	F _c	h ₁	k ₁	l ₁	h	k	l	F _o	F _c	h ₁	k ₁	l ₁
4	0	6	9	-10	4	4	6	0	6	7	21	-22	6	6	7	1	0	9	14	14	1	1	9
3	0	6	20	-21	3	3	6	0	7	7	0	3	7	7	7	2	0	9	0	0	2	2	9
2	0	6	0	6	2	2	6	0	8	7	19	18	8	8	7	3	0	9	10	-9	3	3	9
1	0	6	17	-17	1	1	6	0	9	7	20	18	9	9	7	4	0	9	12	-11	4	4	9
0	0	6	7	-6	0	0	6	0	12	7	10	-13	12	12	7	5	0	9	0	8	5	5	9
1	0	6	0	5	1	1	6	0	14	7	14	17	14	14	7	0	1	9	10	7	1	1	9
2	0	6	0	5	2	2	6	0	8	8	10	-10	8	8	8	0	2	9	9	-12	2	2	9
3	0	6	0	-7	3	3	6	0	5	8	0	0	5	5	8	0	3	9	24	-25	3	3	9
4	0	6	0	-6	4	4	6	0	4	8	0	7	4	4	8	0	4	9	5	-1	4	4	9
5	0	6	0	7	5	5	6	0	3	8	0	-2	3	3	8	0	5	9	15	15	5	5	9
6	0	6	18	-14	6	6	6	0	2	8	10	-12	2	2	8	0	6	9	0	4	6	6	9
7	0	6	0	7	7	7	6	0	1	8	16	-17	1	1	8	0	7	9	6	7	7	7	9
8	0	6	20	15	8	8	6	0	0	8	14	-15	0	0	8	0	8	9	16	-19	8	8	9
0	1	6	29	-30	1	1	6	0	0	8	20	26	0	0	8	0	9	9	9	-6	9	9	9
0	2	6	10	10	2	2	6	7	0	8	18	19	7	7	8	0	3	10	0	6	3	3	10
0	3	6	4	-3	3	3	6	6	0	8	0	-4	6	6	8	0	2	10	0	3	2	2	10
0	4	6	13	-14	4	4	6	5	0	8	0	-6	5	5	8	0	1	10	7	-1	1	1	10
0	5	6	12	14	5	5	6	4	0	8	0	-1	4	4	8	8	0	10	9	-6	8	8	10
0	6	6	7	-4	6	6	6	3	0	8	14	15	3	3	8	7	0	10	17	-21	7	7	10
0	7	6	6	1	7	7	6	2	0	8	14	-14	2	2	8	5	0	10	11	8	5	5	10
0	8	6	6	-6	8	8	6	1	0	8	12	11	1	1	8	4	0	10	15	14	4	4	10
0	9	6	0	4	9	9	6	0	0	8	20	21	0	0	8	3	0	10	0	-7	3	3	10
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0	8	7	6	9	8	8	7	2	0	8	14	-10	2	2	8	1	0	10	11	8	1	1	10
0	5	7	20	-22	5	5	7	3	0	8	0	-4	3	3	8	0	0	10	12	-13	0	0	10
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9	0	7	0	3	9	9	7	0	2	8	14	-15	2	2	8	0	1	10	7	7	1	1	10
8	0	7	14	15	8	8	7	0	3	8	6	8	3	3	8	0	2	10	12	9	2	2	10
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0	2	7	8	8	2	2	7	0	3	9	27	-31	3	3	9	0	5	11	7	6	5	5	11
0	3	7	29	31	3	3	7	0	2	9	16	-15	2	2	9	1	0	12	13	-8	1	1	12
0	4	7	15	17	4	4	7	1	0	9	9	2	1	1	9								
0	5	7	33	-37	5	5	7	0	0	9	21	20	0	0	9								

the standard deviation can not be considered isotropic. The program calculates σ_x , σ_y and σ_z , therefore, and combines these to give σ_{xyz} by

$$\sigma_{xyz}^2 = (\sigma_x a)^2 + (\sigma_y b)^2 + (\sigma_z c)^2. \tag{2}$$

This automatically results in a higher standard deviation than would be obtained using a single value in any given direction. In order to

Table 4. *Final interatomic distances and angles for the Pontiskalk microcline*

T ₁ (0)		T ₁ (m)		T ₂ (0)		T ₂ (m)		K—O	
Interatomic distances									
O _A (1)	1.757 Å	O _A (1)	1.588 Å	O _A (2)	1.620 Å	O _A (2)	1.635 Å	O _A (1)	2.876, 2.890 Å
O _B (0)	1.719	O _B (m)	1.627	O _B (0)	1.586	O _B (m)	1.591	O _A (2)	2.743, (3.408)
O _C (0)	1.722	O _C (m)	1.615	O _C (m)	1.629	O _C (0)	1.613	O _B (0)	2.961
O _D (0)	1.741	O _D (m)	1.623	O _D (m)	1.641	O _D (0)	1.598	O _B (m)	(3.139)
Mean	1.735		1.613		1.619		1.609	O _C (0)	2.923
								O _C (m)	(3.338)
								O _D (0)	2.903
								O _D (m)	2.979

	in T ₁ (0)	in T ₁ (m)	in T ₂ (0)	in T ₂ (m)	σ(<i>d</i>)		
					from σ _m	from σ _{xyz}	
O _A —O _B	2.757 Å	2.607 Å	2.661 Å	2.602 Å	σ(K—O)	0.012 Å	0.018 Å
O _A —O _C	2.924	2.659	2.557	2.576	σ(T—O)	.012	.019
O _A —O _D	2.775	2.570	2.627	2.629	σ(O—O)	.016	.025
O _B —O _C	2.866	2.653	2.639	2.645			
O _B —O _D	2.845	2.679	2.685	2.626			
O _C —O _D	2.815	2.636	2.686	2.678			
Mean	2.830	2.634	2.643	2.626			

	in T ₁ (0)	in T ₁ (m)	in T ₂ (0)	in T ₂ (m)		
Interatomic angles						
O _A —T—O _B	104.94°	108.38°	112.12°	107.51°	T ₁ (0)—O _A (1)—T ₁ (m)	144.30°
O _A O _C	114.39	112.24	103.77	104.95	T ₂ (0)—O _A (2)—T ₂ (m)	138.05
O _A O _D	105.02	106.35	107.30	108.84	T ₁ (0)—O _B (0)—T ₂ (0)	150.90
O _B O _C	112.79	109.83	110.26	111.27	T ₁ (m)—O _B (m)—T ₂ (m)	156.75
O _B O _D	110.66	111.00	112.60	110.93	T ₁ (0)—O _C (0)—T ₂ (m)	131.09
O _C O _D	108.75	109.02	110.40	113.00	T ₁ (m)—O _C (m)—T ₂ (0)	131.87
Mean	109.43	109.47	109.41	109.42	T ₁ (0)—O _D (0)—T ₂ (m)	139.67
					T ₁ (m)—O _D (m)—T ₂ (0)	141.58
					Mean	141.78

make our results comparable with those of investigations in the literature for which the standard deviation is given in only one direction, we list in Table 2 the values of σ_m , the maximum standard deviation in any direction for each atom. The standard deviations of bond lengths in Table 4 have been calculated using both σ_{xyz} and σ_m .

Degree of order

SMITH and BAILEY¹⁸ have proposed new standard values of 1.61 Å and 1.75 Å for tetrahedral Si—O and Al—O distances, respectively, in feldspars. We have applied similar criteria to the tetrahedral O—O distances, and have obtained standard values of 2.62₅ Å and 2.85₅ Å for Si and Al tetrahedra, respectively. The Pontiskalk tetrahedral compositions indicated by linear extrapolation between these standard values are listed in Table 5. Most of the Al has segregated into the T₁(0) site. Using the equation of MACKENZIE and SMITH¹⁹, the degree of order is about 86% for the Pontiskalk microcline, as contrasted to 92% for the Pellotsalo maximum microcline of BROWN and BAILEY⁷.

Table 5. *Tetrahedral Al contents*

	Al from T—O graph	Al from O—O graph
T ₁ (0)	0.90	0.89
T ₁ (<i>m</i>)	.02	.04
T ₂ (0)	.06	.08
T ₂ (<i>m</i>)	.00	.01
ΣAl	0.98	1.02
Degree of order (ΣAl adjusted to 1.00)	89%	83%

The standard error of the mean for the T—O distances, $\sigma_n = \sigma(\text{T—O})/\sqrt{n}$, is 0.006 Å for all four tetrahedra. The standard deviation for testing the significance of the mean distances, therefore, is $\sigma = \sqrt{2} \cdot \sigma_n = 0.008_5$ Å. The difference between the mean T—O distance for T₁(0) and that of each of the other three tetrahedra is highly significant, $\Delta \geq 13.4\sigma$, but the differences between the mean T—O distances for the three small tetrahedra are not significant. A similar result is obtained for the mean O—O distances, here $\Delta \geq 18.6\sigma$ for the differences between T₁(0) and the other tetrahedra. In all of these calculations σ_m has been used rather than σ_{xyz} .

The tetrahedral compositions and degree of order found for the Pontiskalk microcline fit well with the results of previous structural studies of potassic feldspars and with the observed optical properties

¹⁸ J. V. SMITH and S. W. BAILEY, Second review of Al—O and Si—O tetrahedral distances. *Acta Crystallogr.* **16** (1963) 801—811.

¹⁹ W. S. MACKENZIE and J. V. SMITH, Experimental and geological evidence for the stability of alkali feldspars. *Inst. "Lucas Mallada" Cursos y Conf.* **8** (1961) 53—69.

of these specimens. In Fig. 1 a set of smooth curves has been drawn through the points representing the individual tetrahedral Al contents as plotted according to the relative degree of order of each specimen. Likewise, a smooth curve in Fig. 2 relates degree of order to the optic angle $2V$ for all specimens. The graph is non-linear in that $2V$ changes

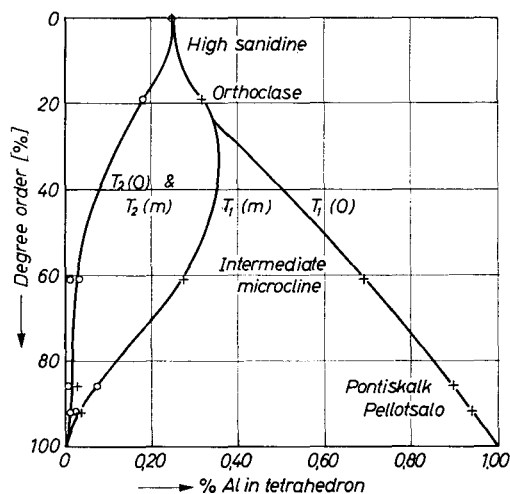


Fig. 1. Al contents of the tetrahedral sites for type specimens of different degrees of Si-Al order. The Al contents were derived from the T—O bond-length graphs of SMITH and BAILEY¹⁸. The equation for the degree of order is given by MACKENZIE and SMITH¹⁹

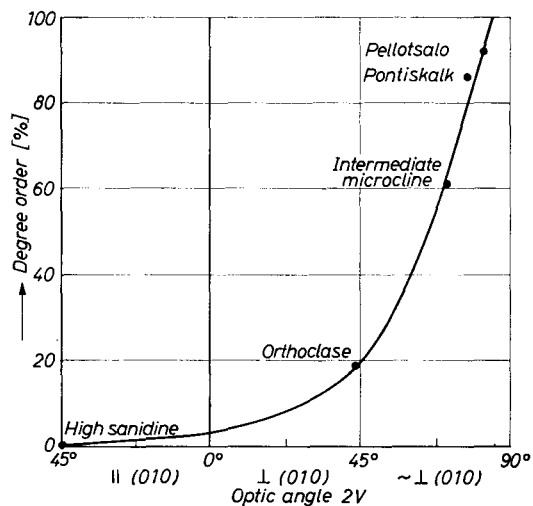


Fig. 2. Variation of optic angle with degree of Si—Al order for type specimens

by 89° in going from high sanidine to orthoclase, a change of 19% in degree of order, but only changes by an additional 41° to reach 100% order. HEWLETT²⁰ has suggested that the birefringence “b” - α,

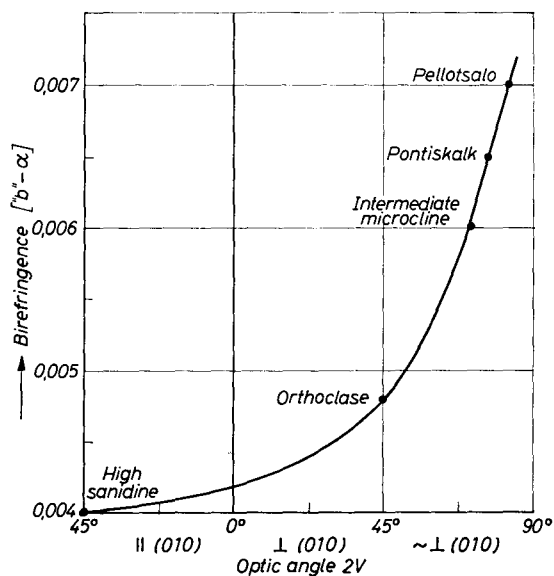


Fig. 3. Variation of birefringence (“b” - α) with optic angle for type specimens

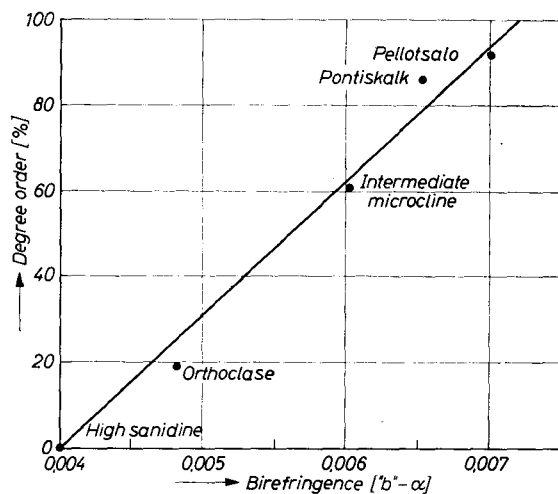


Fig. 4. Variation of birefringence (“b” - α) with degree of Si-Al order for type specimens

²⁰ C. G. HEWLETT, Optical properties of potassic feldspars. Bull. Geol. Soc. Amer. 70 (1959) 511-538.

should be used as a measure of degree of order, where "b" is the refractive index whose vibration direction is most nearly parallel to the *b* axis (γ for microcline and orthoclase and β for high sanidine). Figures 3 and 4 demonstrate that the birefringence varies smoothly with $2V$ and that it is more nearly linear with degree of order than is the optic angle.

It has been assumed, prior to detailed structure determination, that the degree of Si—Al order increases in some regular manner with increasing obliquity, $2V$, birefringence, and extinction angle on (001). The diagrams of BROWN¹¹ and Figs. 1 to 4 of this paper now permit a more quantitative correlation of these parameters. The degree of Si—Al order and the distribution of Al between the tetrahedra can be inferred within certain limits from these diagrams using only a few simple x-ray or optical measurements. The diagrams should not be interpreted too rigorously, however, at this stage of our knowledge. For example, it is important for specimens of intermediate degrees of order that the same ordering path has been followed as in the type specimens. Specimens with unusual geologic histories or with abnormal optic indicatrix orientations may be suspect from this point of view. Corrections for the effect of composition on the optical and geometric parameters (HEWLETT²⁰) may be needed for certain specimens before attempting to evaluate the degree of Si—Al order. Even the type specimens are not exactly comparable compositionally, the Na—Ca feldspar in solid solution ranging from 0 to 2% in the Pontis-kalk microcline to 8 to 9% in orthoclase and sanidine.

MARFUNIN²¹ has claimed that the degree of Si—Al order found by x-ray study by BAILEY and TAYLOR⁶ for an intermediate microcline (Spencer sample *U*) is not in accord with its optic angle. This misunderstanding has arisen because MARFUNIN used a value of 0.32 for the degree of order of the specimen, which is considerably lower than the true value, and a value of 76° for $2V$, slightly higher than the actual optic angle. The degree of order for intermediate microcline should be 0.61 according to the revised standard values of SMITH and BAILEY¹⁸ for tetrahedral Si—O and Al—O distances and the equation of MACKENZIE and SMITH¹⁹. SPENCER²² gives a $2V$ value of 76° for

²¹ A. S. MARFUNIN, The relation between structure and optical orientation in potash-soda feldspars. Inst. "Lucas Mallada" Cursos y Conf. 8 (1961) 97—109.

²² E. SPENCER, The potash-soda feldspars. 1. Thermal stability. Mineral. Mag. 24 (1937) 453—494.

his sample *U*. The crystal chip used in the structure determination was cut from a larger crystal sent from SPENCER to S. W. BAILEY in 1950. Our measurements show a range in $2V$ from 69° to 72° in this crystal, but no values as large as 76° . In Figs. 2 to 3 we have plotted the specimen at 70.5° , the middle of the observed range of $2V$ values, where it agrees well with the degree of order determined by x-ray analysis.

MARFUNIN²¹ has attempted to reconcile the apparent discrepancy between the degree of order and the optic angle of Spencer *U* by proposing that the specimen is twinned on a sub-x-ray scale. He states that in such a case the x-ray structure analysis would not yield the true degree of Si—Al order, which would be given instead by the optic angle. MARFUNIN also states that such examples of sub-x-ray and submicroscopic twinning in K feldspars are common and that they can be recognized by their abnormal orientations of the optic indicatrix. This type of explanation is not necessary for the SPENCER *U* specimen because Figs. 2 to 4 illustrate good agreement between the degree of order and the optical parameters. Although sub-x-ray twinning may be possible in other K feldspars, we believe that the optic orientation variations attributed to this cause by MARFUNIN could be explained equally well as a result of incomplete ordering along atypical ordering paths. A distribution of Al different from that illustrated in Fig. 1 for intermediate microcline, for example, would necessitate a local rearrangement of the oxygen framework of the structure because of the changed sizes of the four tetrahedral sets. This, in turn, should change the orientation of the optic indicatrix.

JONES and TAYLOR⁵ observed a significant difference between the T_1 and T_2 peak heights in the final $[\bar{1}10] F_0$ electron-density map for orthoclase. The difference was in the right direction to correspond to a higher proportion of Al in the T_1 tetrahedron, but the magnitude of the difference was much larger than expected for the small degree of ordering indicated by the T—O bond lengths. Two-dimensional F_0 syntheses constructed by these authors for intermediate microcline and for high sanidine showed a similar reduction in peak height for the T_1 tetrahedra relative to the T_2 tetrahedra for the partly ordered intermediate microcline and identical peak heights for the disordered sanidine. Examination of three-dimensional sections and lines for intermediate microcline by S. W. BAILEY showed an approximate linear decrease of peak height with increasing Al content for the four tetrahedral sets. The sections also showed 20% greater widths in the

XY plane for the Al-rich tetrahedra, a difference not visible on two-dimensional maps.

Electron-density projections were calculated for the Pontiskalk microcline along $[100]$ and $[010]$ of the primitive cell, which correspond to the zones $[110]$ and $[\bar{1}10]$ of the centered cell (Fig. 5). Analysis of these maps (Table 6) indicates an 8% reduction in peak height for the Al-rich site, $T_1(0)$, but no significant difference in peak width. The magnitude of the reduction in peak height is consistent with that found for intermediate microcline, considering their relative degrees of

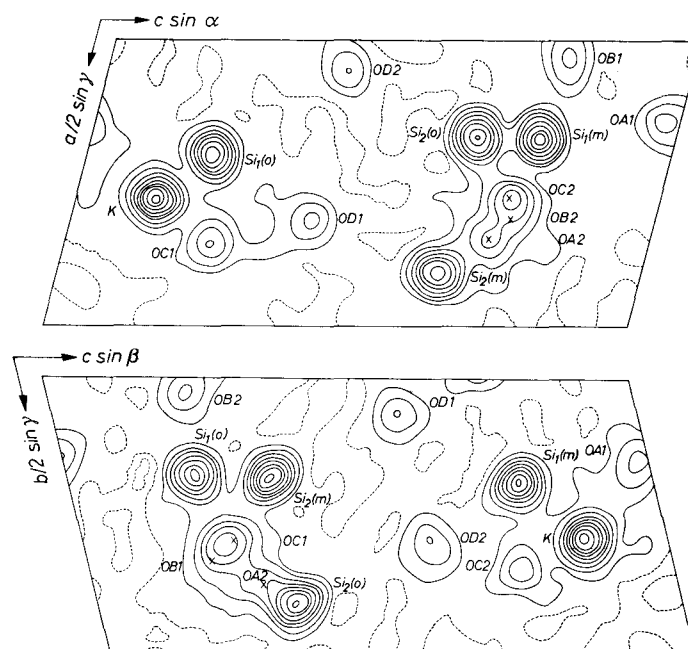


Fig. 5. Electron-density projections along $[010]$ (upper map) and $[100]$ (lower map) zones of primitive cell. Contour interval $5 e/\text{\AA}^2$. Zero and negative contours are dashed

Table 6. *Electron-density peak values for the tetrahedral sites from $[100]$ and $[010]$ projections*

	Peak heights			Peak widths (arbitrary units)		
	$[100]$	$[010]$	Mean	$[100]$	$[010]$	Mean
$T_1(0)$	$36 e/\text{\AA}^2$	$39 e/\text{\AA}^2$	$37.5 e/\text{\AA}^2$	37	38	37.5
$T_1(m)$	40	42	41	37	38	37.5
$T_2(0)$	40	41	40.5	—	39	39
$T_2(m)$	41	39	40	39	39	39

Si—Al order, but is much smaller percentagewise than would be expected from the results for orthoclase alone.

The observed differences in peak heights are probably related not so much to the difference in electron content of the tetrahedral sites as to their effective temperature factors. The effective temperature factors provide measures of the amount of thermal vibration and disorder for these sites in the structure, of the quantity and accuracy of the experimental data, and of the validity of the scattering factors used in the calculation of phases. BROWN and BAILEY⁷ have shown for the Pellotsalo microcline that the effective temperature factors determined by the least-squares method are strongly dependent on the scattering factors used. The use of f_{Si} for all four tetrahedral sites resulted in a temperature factor for the Al-rich site approximately twice that of the Si-rich sites. The same effect was noted during the first stage of refinement for the Pontiskalk microcline. Use of f_{Al} for site T₁(0) and f_{Si} for the other three tetrahedral sites in the second and third stages of refinement resulted in B values approximately the same for all four sites (Table 2). For orthoclase, JONES and TAYLOR⁵ have discussed the possibility that the relatively large observed peak-height difference may be indicative of an "average" structure either for the several cells over which the Si—Al is partly ordered, for a sub-x-ray twinned microcline, or for a doubled unit cell obscured by stacking faults or small anti-phase domains.

Potassium atom

Of the ten closest oxygen neighbors to potassium in the Pontiskalk microcline, seven have K—O contacts under 3.00 Å (Table 4) and are considered to be in the primary coordination group. Atoms O_B(m) at a distance of 3.139 Å, O_C(m) at 3.338 Å, and O_A(200 c) at 3.408 Å are farther away from the potassium and are considered to be outside its primary coordination. This arrangement is almost identical to that found in the Pellotsalo microcline. For this reason local charge-balance calculations for the two microclines are the same. It is also noted in both maximum-microcline structures that the oxygens in the Al-rich tetrahedron tend to be closer to the potassium, on the average, than are the other oxygens, whose negative charges are already satisfied by their bonds to two silicons. There is no noticeable effect of the number of close K neighbors on individual T—O bond lengths in the Pontiskalk microcline.

The orientation of the anisotropic thermal ellipsoid for potassium (Table 7) is approximately the same as in the Pellotsalo microcline. The principal axes deviate at most by 19° for the two specimens, but with positional errors up to 18° for the Pontiskalk microcline and up to 10° for the Pellotsalo microcline so that there is overlap between the volumes of most probable axis orientations. The greatest difference is in the relative lengths of the ellipsoid axes for the two specimens. The major axes are approximately the same in length and direction. The minor ellipsoid axis of the Pontiskalk microcline, however, is parallel to the median ellipsoid axis of the Pellotsalo microcline.

Table 7. *Anisotropic thermal ellipsoid for potassium*

Ellipsoid axis	r.m.s.	B	Angles to crystal axes		
			X	Y	Z
1	0.100 ± 14	0.79 ± 22	$80^\circ \pm 16^\circ$	$51^\circ \pm 7^\circ$	$52^\circ \pm 7^\circ$
2	0.131 ± 7	1.35 ± 15	$31^\circ \pm 16^\circ$	$116^\circ \pm 18^\circ$	$102^\circ \pm 9^\circ$
3	0.163 ± 12	2.10 ± 32	$119^\circ \pm 12^\circ$	$130^\circ \pm 9^\circ$	$40^\circ \pm 6^\circ$

No structural interpretation has been found for the observed vibration-displacement differences along the minor and median ellipsoid axes for the two microclines, even though the differences are greater than the calculated errors. It is noted that the isotropic B values for the oxygen atoms in the Pontiskalk microcline show twofold greater variability than in the Pellotsalo microcline. For example, B for oxygen ranges from 0.58 to 1.42 in the Pontiskalk specimen and from 0.67 to 1.03 in the Pellotsalo specimen. This may indicate greater disorder in the positions of the Pontiskalk oxygens because of the low temperature of formation. On the other hand, it is also possible that the errors due to the smaller amount of experimental data used for the Pontiskalk specimen may have been absorbed in the individual B values by the least-squares method of refinement. The same reasoning can be applied to the potassium anisotropic B values. LONSDALE and MILLEDGE²³ have illustrated the danger of overemphasizing the significance of thermal parameters. They refined two independent and apparently reliable sets of data for the same compound and derived two sets of thermal ellipsoids even more discordant than the examples cited here for microcline.

²³ K. LONSDALE and J. MILLEDGE, Analysis of thermal vibrations in crystals: a warning. *Acta Crystallogr.* 14 (1961) 59–61.

Comparison of Pontiskalk and Pellotsalo microclines

According to the accuracy of the results the difference between the degree of Si—Al order found in this investigation (86%) and that found by BROWN and BAILEY⁷ for the Pellotsalo maximum microcline (92%) is not statistically significant, $\Delta = 0.8\sigma$. The difference from 100% order is possibly significant²⁴, $\Delta = 1.9\sigma$. The similarity between the two structures of maximum microcline is emphasized by a comparison of the results of this investigation with the results for the Pellotsalo microcline at the end of its first stage of refinement, which included a similar number of reflections and should be of comparable accuracy. This comparison (Table 8) shows that the mean change in the T—O bond lengths for the Pellotsalo microcline from the end of the first refinement stage (600 reflections) to the final results (2,341 reflections) is 0.012 Å, whereas the mean difference between the Pontiskalk and Pellotsalo final T—O bond lengths is 0.013 Å. This indicates that it

Table 8. Comparison of tetrahedral bond-length differences at different refinement stages of the Pellotsalo and Pontiskalk microclines

A = Pellotsalo first refinement stage

B = Pellotsalo final refinement

C = Pontiskalk final refinement

	<i>A</i> — <i>B</i>	<i>B</i> — <i>C</i>
T ₁ (0)—O _A (1)	0.008 Å	0.019 Å
O _B (0)	.018	.020
O _σ (0)	.027	.023
O _D (0)	.024	.000
T ₁ (<i>m</i>)—O _A (1)	.010	.004
O _B (<i>m</i>)	.004	.019
O _σ (<i>m</i>)	.011	.014
O _D (<i>m</i>)	.006	.004
T ₂ (0)—O _A (2)	.004	.006
O _B (0)	.024	.012
O _σ (<i>m</i>)	.004	.004
O _D (<i>m</i>)	.015	.020
T ₂ (<i>m</i>)—O _A (2)	.001	.009
O _B (<i>m</i>)	.001	.026
O _σ (0)	.019	.020
O _D (0)	.013	.006
Mean differences	0.012	0.013

²⁴ D. W. J. CRUICKSHANK, The accuracy of electron-density maps in x-ray analysis with special reference to dibenzyl. *Acta Crystallogr.* **2** (1949) 65—82.

is quite possible that the structure of the Pontiskalk microcline would converge to that of the Pellotsalo microcline upon further refinement with a comparable number of reflections.

Despite the lack of statistical significance for a difference between the two maximum microcline structures, the good fit of the points in Figs. 1 to 4 suggests that the relative degrees of order found for the two specimens may be correct. The optical parameters that are sensitive to degree of order, such as $2V$, total birefringence, and extinction on (001), all suggest that the Pontiskalk authigenic microcline is slightly less ordered than the Pellotsalo igneous microcline. The geometrical parameters, obliquity value and γ^* , are nearly identical for the two specimens, however, and for all practical purposes the Pontiskalk authigenic microcline exists in the same highly ordered state as the Pellotsalo granitic microcline.

There are two important differences between granitic and authigenic microclines. Firstly, except for two occurrences reported by BÖGGILD²⁵ and BARTH²⁶, granitic microclines exhibit monoclinic morphology and are usually twinned in the familiar cross-hatch pattern. These microclines appear to be secondary in the sense that they crystallized originally at moderate to relatively high temperatures as monoclinic, disordered phases and inverted during cooling by a diffusive, ordering transformation. BROWN¹¹ and BROWN and BAILEY⁷ have explained the cross-hatch twinning as a natural consequence of the Al ordering into either the $T_1(0)$ or the equally favorable $T_1(m)$ tetrahedron in different domains of the crystal. Authigenic microclines, in contrast, are characterized by triclinic morphology and lack of cross-hatch twinning. They appear to have crystallized directly as the ordered phase at a low temperature within the stability field of microcline. Secondly, granitic microclines are normally perthitic. Unmixing of a Na-rich phase from an original homogeneous K—Na solid solution took place during the same cooling history that produced ordering of Si—Al. Authigenic microclines are never perthitic and are essentially soda-free, undoubtedly as a result of their low temperature of crystallization.

The primary microcline described by BARTH²⁶ occurs in a chlorite schist from Stöa, Norway. It is a homogeneous, non-perthitic specimen

²⁵ O. B. BÖGGILD, Über die Krystallform des Mikroklins. *Z. Kristallogr.* **48** (1911) 466–472.

²⁶ T. F. W. BARTH, The interrelations of the structural variants of the potash feldspars. *Z. Kristallogr.* **112** (1959) 263–274.

of composition $\text{Or}_{97}\text{Ab}_3$ and obliquity $\Delta = 0.93$. The only twins present are large, irregular units with irrational boundaries. A temperature of crystallization of 270°C was determined for the specimen by the feldspar geologic thermometer method (BARTH²⁷). Based partly on this result, BARTH²⁶ has set an upper limit of 300°C for the stability field of maximum microcline. Authigenic feldspars must crystallize well below this upper limit. Present knowledge indicates that the temperature of sediments under load does not exceed 160°C . BASKIN² set 100°C as a maximum temperature of formation in his survey of authigenic feldspars.

The Pontiskalk limestone does not show any evidence of thermal metamorphism, but has been dolomitized. BASKIN² states that all the carbonate rocks containing authigenic feldspar crystals that he examined had been partly or completely dolomitized. It is quite possible that the Pontiskalk microcline crystals were formed during the reorganization associated with the dolomitization, which is here considered part of the diagenetic history of the rock rather than being hydrothermal or metamorphic.

Although the Pontiskalk and Pellotsalo maximum microclines crystallized in different geologic environments at temperatures probably several hundred degrees apart, their unit cell parameters, optical properties, atomic positions, bond lengths, and degrees of Si—Al order are extremely similar. Only the temperature factors show any appreciable differences. Instead of approaching the ordered state by a diffusive transformation during cooling, like the Pellotsalo microcline, the Pontiskalk microcline is believed to have crystallized *within* the stability field of the fully ordered phase because of the evidence of the geologic occurrence, the euhedral triclinic morphology, and the unique fourling twins. There is, however, no resulting structural difference between the authigenic and igneous maximum microcline specimens. Essentially complete Si—Al ordering has been achieved by the authigenic microcline without the benefit of appreciable thermal mobility, probably as a result of a very slow growth rate and a hydrous environment. Composition may also have been a factor. SMITH and MACKENZIE¹⁰ suggest that a pure K feldspar should order more easily than one containing a few percent Na feldspar in solid solution. The fact that

²⁷ T. W. BARTH, Studies in gneiss and granite: I. Relation between temperature and the composition of the feldspars. *Skrifter Norske Vidensk. Akad., Mat.-nat. Kl. 1* (1956) 3—16.