X-RAY AND OPTICAL STUDY OF ALKALI FELDSPAR: II. AN X-RAY METHOD FOR DETERMINING THE COMPOSITION AND STRUCTURAL STATE FROM MEASUREMENT OF 2θ VALUES FOR THREE REFLECTIONS.[1]

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ABSTRACT

Measured 2θ values of the $\overline{2}01$, 060, and $\overline{2}04$ diffraction peaks of natural and synthetic alkali feldspars empirically can be linearly related to the a, b, and c cell parameters, respectively. The structural state of many alkali feldspars may be estimated directly from a plot of 2θ (060) against 2θ ($\overline{2}04$) prepared for feldspars of known structural state. Feldspars having anomalous cell dimensions may also be recognized on such a plot. Composition of feldspars having normal cell dimensions may be determined from 2θ ($\overline{2}01$). Starting parameters for a computer refinement of the cell may be obtained from equations relating cell dimension to 2θ value of a single diffraction peak for a wide variety of natural, synthetic, and cation-exchanged alkali-feldspar phases. The 'three-peak' method permits any geologist who has access to an X-ray diffractometer to describe and name alkali feldspar phases commonly encountered in petrologic studies.

INTRODUCTION

In a preceding paper (Wright and Stewart, 1968; Part I of this study), a method was described by which composition and structural state of alkali feldspar could be determined from cell dimensions refined by computer using powder X-ray diffraction data. While processing the computed results, certain distinctive and ubiquitous feldspar reflections were found whose 2θ values depended principally on a *single* unit-cell dimension. Discovery of such reflections suggested the possibility of using the 2θ values instead of cell parameters to estimate structural state and composition of natural alkali feldspars. The three most useful reflections and the cell parameter on which their 2θ value depends are $\overline{2}01$—a, 060—b, and $\overline{2}04$—c. The reflections are commonly of sufficient intensity to be accurately measured and indexed from diffraction patterns of alkali feldspars collected from a wide variety of geological environments. Best fit curves relating the 2θ values to the appropriate cell dimension are essentially linear and permit easy estimation of starting parameters for a complete refinement of the unit cell. The sections following describe this 'three-peak' method of studying alkali feldspars in some detail.

METHODS OF STUDY

The 2θ values and cell dimensions that form the basis for the 'three-

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peak' method are abstracted from the data for synthetic, base-exchanged, and natural alkali feldspars compiled in Part I.

Methods of measurement are described in the appendix of that paper. Cell dimensions were obtained using the computer program of Evans, Appleman, and Handwerker (1963) with subsequent modifications by Appleman and Handwerker. Equations relating cell dimension to 2θ value were computed using a standard least-squares program.

Identification of reflections. The approximate ranges of 2θ (CuKα_1) for five reflections that are used in the 'three-peak method' are listed in Table 1. (See also Tables 11–15, Part I). The $\bar{2}01$ and 060 reflections may be indexed unambiguously in all natural alkali feldspars. The $\bar{2}04$ is a strong, single reflection in most orthoclase, microcline, anorthoclase,

TABLE 1. POSITION OF ALKALI FELDSPAR REFLECTIONS USED IN
'THREE-PEAK' REFINEMENT

Miller Indices, hkl	Approximate Intensity	Approximate Range of 2θ (CuKα_1)		
		Potassium-rich phases	Anorthoclases	Albite
($\bar{2}$01)	40	20.8°–21.2°	21.6°–21.9°	21.9°–22.1°
(002)	>100	27.4°–27.8°	27.8°–28.0°	27.9°–28.1°
($\bar{1}$13)	8	38.6°–39.0°	not present	not present
(060)	25	41.6°–42.0°	41.7°- 42.0°	42.2°–42.6°
($\bar{2}$04)	30	50.5°–51.1°	51.1°–51.3°	51.2°–51.5°

and albite samples. In sanidine or orthoclase having anomalous cell dimensions $\bar{2}04$ is commonly either overlapped by or joined by one or more additional reflections. If reflections in the vicinity of $\bar{2}04$ are sharp, 2θ values of the $\bar{1}13$ and 002 reflections may be used to make an unambiguous identification of the reflection whose index is $\bar{2}04$, as shown in Figure 1.

PRESENTATION OF DATA

2θ values for 060 and $\bar{2}04$ are plotted against one another in Figures 2 and 3 for the three complete series of feldspars and for most of the other cation-exchanged feldspars reported on by Orville, (1967) and in Part I. The presentation is analogous to the $b-c$ plots of the latter paper (Figs. 2a and 2b). The data from which Figures 2 and 3 are constructed are given in Table 3. 2θ values for SynSanShaw, P50—90 KF, and their exchange equivalents are given in Table 3 but not plotted on Figure 3 as

the former was shown to have anomalous cell dimensions and the latter
has considerable Ba and Sr in its bulk composition (see Part I). For the
three complete feldspar series 2θ values of $\overline{2}01$ are plotted against Or
content in Figure 4, which can be compared with the plot of a against Or
content for these same series (Part I, Fig. 1a). Equations relating 2θ
value of $\overline{2}01$ to Or content are given in Table 4.

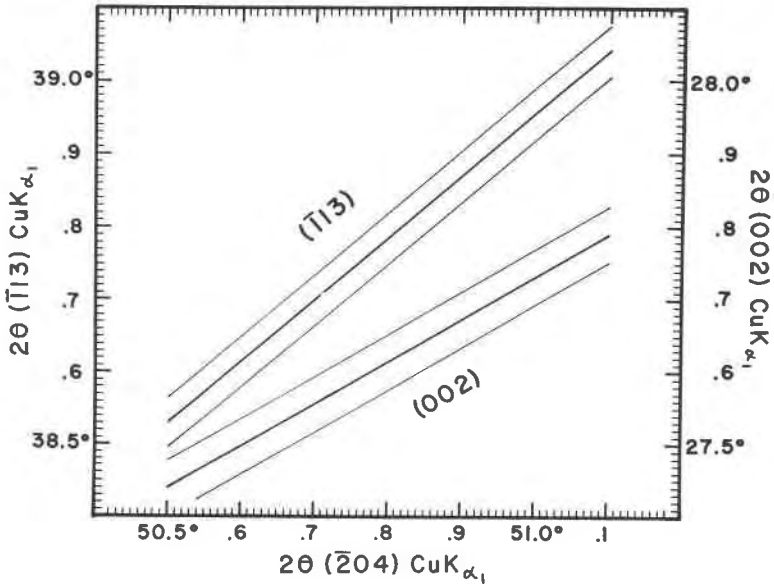Equations relating 2θ value of a single diffraction peak to the appropri-

FIG. 1. Plotted lines that enable identification of $\overline{2}04$ where more than one reflection
occurs between 50° and 51° 2θ, CuKα_1. The upper line relates the position of the $\overline{1}13$ and $\overline{2}04$
reflections, according to the relationship 2θ $(\overline{2}04) = 1.1780$ $[2\theta$ $(\overline{1}13)] + 5.1048 \pm 0.0202°$ 2θ
$(\overline{2}04)$. The lower curve relates the position of the 002 and $\overline{2}04$ reflections, according to the
relationship 2θ $(\overline{2}04) = 1.6886$ $[2\theta$ $(002)] + 4.1690 \pm 0.0317°$ 2θ $(\overline{2}04)$. Light boundary lines
are drawn at points corresponding to ± 2 standard deviations of 2θ $(\overline{2}04)$.

ate cell parameter are tabulated and discussed in an Appendix. These
equations demonstrate the linear relationship between 2θ value and cell
dimension and may be used to obtain starting parameters for computer
refinement of the unit cell. Cell dimensions computed from the equations
are not, of course, as accurate as those obtained from a good cell refine-
ment and should not be quoted in comparison with feldspars whose di-
mensions have been so refined.

In the course of tabulating the values of 2θ for $\overline{2}04$, 060, and $\overline{2}01$ it was
discovered that the values calculated by the computer in a cell refine-

ment differed by as much as $\pm 0.03°$ 2θ from the observed values for these reflections. In Table 2 the deviations of calculated from observed 2θ values are summarized for each of the three reflections measured for each complete series. In all but two instances the average absolute deviation
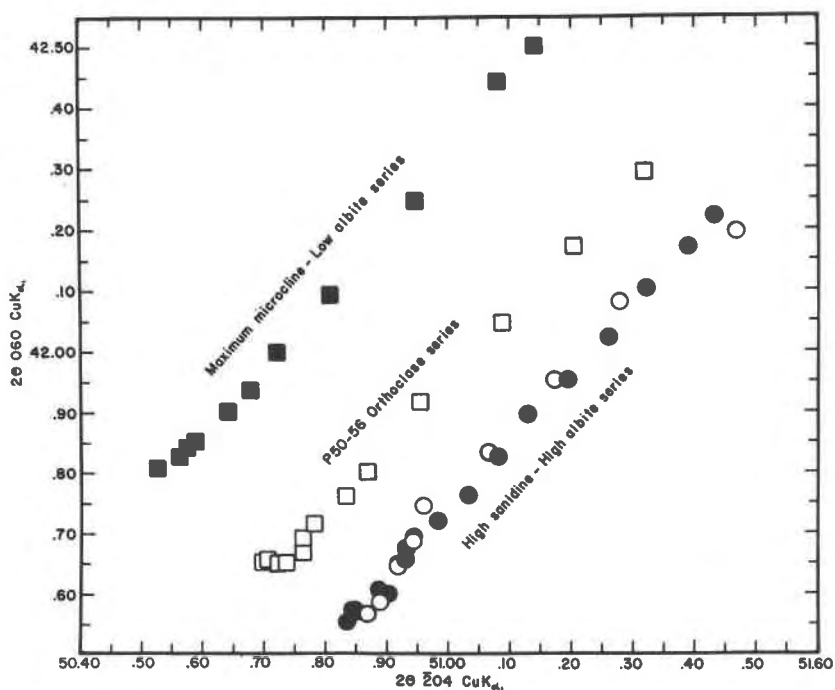

FIG. 2. Observed 2θ values of 060 plotted against observed 2θ values of $\overline{2}04$ for members of three complete series of alkali feldspars reported in Part I.

Solid Squares: Maximum microcline—low albite series, data of Orville (1967).

Open Squares: P50-56F (orthoclase) series, data of Wright and Stewart (1968).

Solid Circles: High sanidine-high albite series, data of Orville (1967).

Open Circles: High sanidine-high albite series, data of Donnay and Donnay (1952 and written communication, 1963).

Data points are drawn to $\pm 0.02°$ 2θ which exceeds the range observed in measurement of three X-ray patterns for each sample.

is less than $\pm 0.01°$ 2θ, well within the error inherent in measurement of the reflection. The average deviations using the signed values of 2θ (observed) minus 2θ (calculated) are also shown in Table 2. Theoretically these average deviations should all be zero for a random deviation of the calculated values around the observed ones. In the actual cases there is always a small bias. For the sake of consistency and maximum applic-
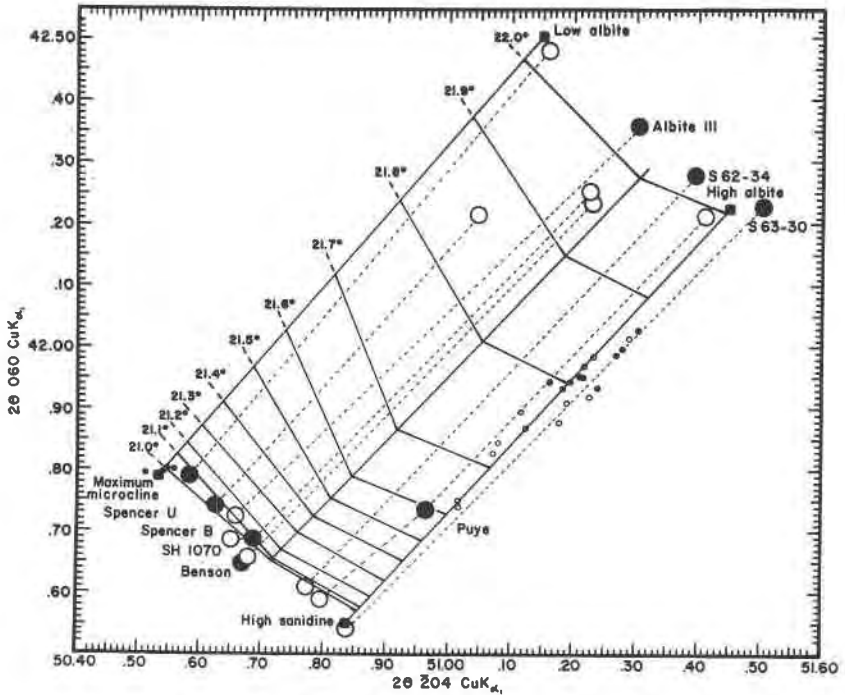
FIG. 3. Alkali exchange paths (see Part I, Fig. 2) on a plot of $2\theta(060)$ against $2\theta(\overline{2}04)$. Solid lines are drawn by eye from the data of Figure 2. Solid squares define the approximate positions of maximum high and low structural states at $NaAlSi_3O_8$ and $KAlSi_3O_8$ bulk composition. Dashed lines connect data for exchanged feldspars studied in Part I. Cross-contours are $2\theta(\overline{2}01)$, interpolated as straight lines between points for the three complete series. Data for natural maximum microclines (Wright and Stewart, unpub. data), and for natural anorthoclases (Carmichael and Mackenzie, 1964, Stewart, unpub. data) are plotted as small circles, for comparison with Part I, Fig. 2.

ability to observations of natural alkali feldspars, the equations of Tables 5 and 6 and the data of Figures 2–4 relate the *observed* 2θ to the appropriate computed cell parameter.

DETERMINATION OF COMPOSITION AND STRUCTURAL STATE OF ALKALI FELDSPAR AND IDENTIFICATION OF 'ANOMALOUS' FELDSPARS USING THE 2θ VALUES FOR $\overline{2}01$, 060, AND $\overline{2}04$

The methods of this section are exactly analogous to those described in Part I (p. 45ff) using the cell dimensions a, b, and c, and the feldspar can also be named and described using terminology given in Part I (p. 33ff). The procedure following the 'three-peak' method is as follows:

1. Measure carefully 2θ values for $\overline{2}01$, 060, $\overline{2}04$, $\overline{1}13$ (if present), and
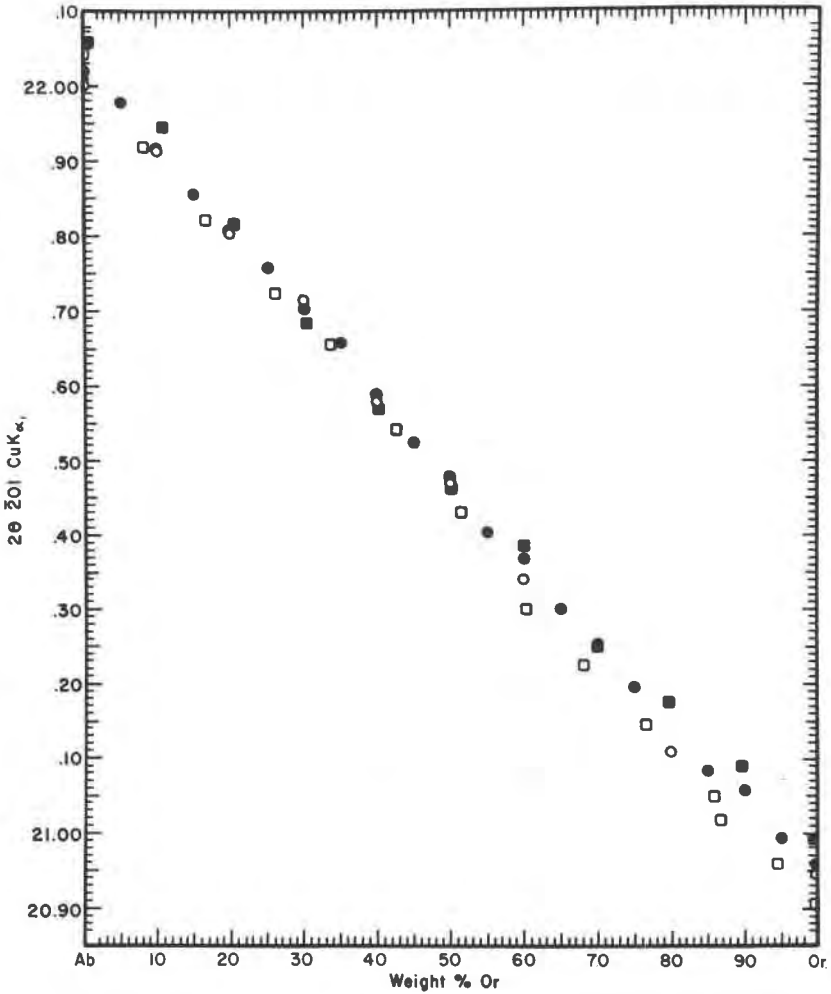
Fig. 4. Or content plotted against $2\theta(\bar{2}01)$ for three complete series of exchanged feldspars. Data sources and symbols as given for Figure 2. Equations relating $2\theta(\bar{2}01)$ to Or content for each series are given in Table 4.

002 using methods described in Part I (Appendix). Refer to Figure 1 to identify $\bar{2}04$ when more than one sharp diffraction peak appears between 50° and 51° 2θ (CuKα_1). In the rare cases where reflections near to and including $\bar{2}04$ are fuzzy the 'three-peak' method is inapplicable.

2. Plot the 2θ values of 060 and $\bar{2}04$ on Figure 3 and read off the approximate 2θ value of $\bar{2}01$ from the contours. If this value agrees within

$0.1°$ 2θ with the 2θ value directly measured for $\overline{2}01$ the feldspar may be assumed to have normal cell dimensions. In cases where the 2θ value of $\overline{2}01$ derived from Figure 3 exceeds the measured value by $0.1°$ 2θ or more then the feldspar may be termed anomalous.

3. For normal feldspars structural state is obtained directly from

TABLE 2. DEVIATIONS OF CALCULATED VALUES FROM OBSERVED
VALUES OF $2\theta(\overline{2}01)$, $2\theta(060)$, AND $2\theta(\overline{2}04)$

Series	Reflection	(2θ observed)−(2θ calculated)[1]				Number of Observations
		Absolute Deviation	Average Absolute Deviation	Signed Deviation	Average Signed Deviations	
High sanidine—	($\overline{2}01$)	.148	.007	+ .014	+0.001	20
high albite	(060)	.090	.0045	− .060	−0.003	20
Orville (1967)	($\overline{2}04$)	.156	.008	− .138	−0.007	20
High sanidine—	($\overline{2}01$)	.054	.006	− .006	−0.0005	9
high albite	(060)	.123	.014	+ .117	+0.012	9
Donnay and Donnay (1952)	($\overline{2}04$)	.047	.010	+ .047	+0.010	5
P50–56 KF	($\overline{2}01$)	.072	.007	− .010	−0.001	10
Orthoclase	(060)	.051	.005	− .005	−0.0005	10
Wright and Stewart (1968)	($\overline{2}04$)	.065	.0065	− .011	−0.001	10
Maximum microcline—	($\overline{2}01$)	.070	.0065	− .010	−0.001	11
low albite	(060)	.051	.005	− .040	−0.004	10
Orville (1967)	($\overline{2}04$)	.041	.004	+ .011	+0.001	11

[1] Differences are calculated as absolute (unsigned) quantities in column 3 and 4. In columns 5 and 6 the signs of the differences are retained. The values in columns 5 and 6 should be zero for perfectly random variation.

Figure 3 in terms of the closest plotted feldspar of known structural state (see example below). Because of the difference in ordering scheme for Na-rich compared with K-rich feldspars, discussed in detail in Part I (p. 27ff), the structural state should be described only in terms of the cation-exchanged feldspar series in which the starting material was nearly the same composition as the unknown. The structural state of natural *albite* and *anorthoclase* should be compared to the equivalents of high albite (including S63-30), S62-34, Albite III, and low albite. The structural state of *potassium-rich feldspars* should be compared to the equivalents for High Sanidine, Puye (=low sanidine), P50-56F, Benson, SH 1070, Spencer B, Spencer U, and maximum microcline.

TABLE 3. DATA USED TO PREPARE FIGURES 2 AND 3.

Feldspar Series	Bulk Composition (Wt. % Or)	Observed 2θ (CuKα_1)[a]		
		$(\overline{2}01)$	(060)	$(\overline{2}04)$
Synthetic high sanidine-	100	20.959	41.577	50.845
high albite	95	20.995	41.558	50.836
(Orville, 1967)	90	21.059	41.577	50.850
	85	21.085	41.575	50.852
	75	21.197	41.598	50.892
	70	21.254	41.611	50.888
	65	21.300	41.605	50.904
	60	21.369	41.652	50.920
	55	21.404	41.659	50.930
	50	21.480	41.680	50.932
	45	21.525	41.696	50.945
	40	21.591	41.722	50.984
	35	21.657	41.764	51.034
	30	21.703	41.828	51.082
	25	21.757	41.896	51.130
	20	21.807	41.954	51.194
	15	21.856	42.023	51.261
	10	21.918	42.103	51.322
	5	21.977	42.171	51.390
	0	22.019	42.222	51.433
Synthetic high sanidine-	100	20.945	41.570	50.870
high albite	80	21.160	41.590	50.890
(Donnay and Donnay 1952)	60	21.340	41.650	50.920
	50	21.470	41.690	50.945
	40	21.580	41.745	50.960
	30	21.715	41.835	51.068*
	20	21.805	41.955	51.175*
	10	21.915	42.080	51.281*
	0	22.000	42.195	51.468*
Orthoclase (P50–56KF)	100 (extrapolated)	20.905*	41.655*	50.700*
(Wright and Stewart 1968)	94.5	20.960	41.653	50.723
	86.8	21.018	41.653	50.738
	85.9	21.051	41.660	50.706
	76.7	21.146	41.651	50.730
	68.3	21.225	41.671	50.766
	60.4	21.301	41.693	50.766
	51.6	21.431	41.716	50.783
	42.8	21.541	41.763	50.835
	34.0	21.655	41.801	50.870
	26.3	21.723	41.916	50.955
	16.8	21.820	42.045	51.090
	8.4	21.918	41.171	51.203
	0 (extrapolated)	22.043*	42.291*	51.320*
Maximum microcline-low	99.5	20.993	41.809	50.527
albite	89.7	21.091	41.829	50.565
(Orville 1967)	79.8	21.176	41.841	50.576
	70.0	21.254	41.853	50.589
	60.1	21.387	41.900	50.642
	50.3	21.465	41.938	50.680
	40.4	21.570	41.999	50.723
	30.6	21.684	42.094	50.810
	20.7	21.815	42.245	50.948
	10.9	21.945	42.441*	51.082
	1.0	22.057	42.500	51.142

TABLE 3—(*continued*)

Feldspar Series	Bulk Composition (Wt. % Or)	(Observed 2θ CuK$_{\alpha i}$)[a]		
		($\bar{2}$01)	(060)	($\bar{2}$04)
SynSanShaw (Wright and	100	20.950	41.583	50.900*
Stewart, 1968, Table 2)	0	22.011	42.206	51.435
S 63-30	0	22.024	42.231	51.504
	100	20.978	41.546	50.838
Puye	42	21.565	41.739	50.964
	95	20.988	41.590	50.796
	2	21.990	42.215	51.411
P50-90	62	21.316	41.618	50.863
	92	20.985	41.571	50.773
	12	21.876	42.076	51.260
Benson	94	20.955	41.653	50.670
	7	21.938	42.237	51.230
	96	20.931	41.659	50.678
SH 1070	87	21.048	41.690	50.690
	94.5	20.961	41.686	50.651
	4	21.960	42.255	51.226
Spencer B	91	21.058	41.743	50.625
	~6	21.927	42.216	51.047
Spencer U	94	20.998	41.792	50.583
	94	20.986	41.766	50.585
	~0	22.020	42.482	51.159
S62-34	~0	22.031	42.282	51.392
	100	20.946	41.610	50.772
Low albite III	0	22.013	42.360	51.303
	100	20.928	41.726	50.657
Natural maximum microclines				
Amicr (Stewart, unpub.)	96	21.003	41.797	50.512
SH 22500 (Wright 1967)	96	21.006	41.803	50.546
MP-3 Mi (Wright, unpub.)	94.2	21.020	41.800	50.543
P63-1 Mi (Do.)	93.3	21.040	41.803	50.560
Natural anorthoclases				

	Or[b]	*Ab*[b]	*An*[b]	*Other*[b]			
AHR 48[c]	19.5	75.6	4.9	—	21.795	41.947	51.197
AHR 35[c]	. . . .			. . .	21.800	41.938	51.240
AHR 50[c]	. . . .			. . .	21.795	41.955	51.212
AHR 42[c]	. . . .			. . .	21.766	41.955	51.218
BTB 8	15.7	74.2	10.1	—	21.850	41.900	51.270
FR-1[c]	16.8	64.8	18.4	—	21.830	42.000	51.280
#1[d]	11.8	76.8	10.7	0.7	21.899	42.030	51.304
#2	14.0	77.4	7.8	0.8	21.866*	42.019*	51.290*
#3	17.8	74.1	6.9	1.2	21.801*	41.972*	51.217*
#4	18.7	71.1	8.9	1.2	21.797*	41.938*	51.233*
#5	18.8	79.1	1.1	1.0	21.808	41.947	51.165
#6	21.2	75.6	2.1	1.0	21.771*	41.880*	51.179*
#7	21.8	75.8	0.9	1.5	21.791*	41.936*	51.185*

TABLE 3—(*continued*)

Feldspar Series					Bulk Composition (Wt. % Or)			Observed 2θ (CuKα_1)[a]	
							$(\bar{2}01)$	(060)	$(\bar{2}04)$
#8	22.5	72.0	4.4	1.1	21.736*	41.913*	51.191*
#9	23.0	69.3	7.4	0.3	21.776*	41.923*	51.227*
#10	23.2	75.2	1.2	0.4	21.741*	41.898*	51.117*
#11	23.3	73.8	1.5	1.3	21.742*	41.871*	51.125*
#12	24.0	65.9	10.1	—	21.696*	41.848*	51.082*
#13	31.7	66.3	1.8	0.2	21.677*	41.753*	51.018*
#14	32.5	61.4	6.1	—	21.694*	41.830*	51.073*
#15	33.0	66.8	0.2	—	21.654*	41.742*	51.018*

[a] Where 2θ was not measured the value calculated from the refinement is given and starred, e.g., 51.068*.
[b] Analyses of specimens.
[c] Stewart, unpub.
[d] Carmichael and Mackenzie (1964, Table II).

Composition of normal feldspars may be obtained from Figure 4 or the equations of Table 4 once structural state is established.

4. For anomalous feldspars the 'apparent' structural state may be derived in the same way as for normal feldspars. It is yet to be established to what extent this will depart from the true structural state (see discussion in Part I (p. 71). Composition *cannot* be obtained from the 2θ value for $\bar{2}01$. However, the appendix tables may be used to derive starting parameters for a cell refinement from which cell volume may be used to estimate composition (Part I, p. 71).

Three samples of alkali feldspar, previously named and described in

TABLE 4. EQUATIONS RELATING 2θ ($\bar{2}01$) (x) AND Or CONTENT (y) FOR COMPLETE SERIES OF ALKALI FELDSPARS OF CONSTANT STRUCTURAL STATE, WHERE $y = mx + b$

Feldspar series	m	b	No. of Observations	Standard error of y[a]	Reference
High sanidine-high albite	−92.18	+2030.05	29	1.17 (3–0.91)	Orville (1967)
P50–56KF (Orthoclase)	−87.69	+1930.77	12	1.37 (3–1.13)	Wright and Stewart (1968)
Maximum microcline-low albite	−92.19	+2031.77	11	2.40 (2–1.08)	Orville (1967)

[a] Where the best fit is not linear the degree and standard error of the best fit polynomial are given in parenthesis, *e.g.* (2–0.0042) indicates the best fit is a quadratic for which the standard error of y is 0.0042

TABLE 5. EQUATIONS RELATING CELL DIMENSIONS TO OBSERVED 2θ VALUES OF SINGLE REFLECTIONS FOR COMPLETE SERIES OF ALKALI FELDSPARS OF CONSTANT STRUCTURAL STATE

Feldspar series	Symmetry and Composition	Variables		Equation, $y=mx+b$		No. of Observations	Standard error of y[a]
		x	y	m	b		
High sanidine–high albite Combined data of Orville (1967) and Donnay and Donnay (1952) re-refined by Wright and Stewart, (1968)	Monoclinic Or≥40	$2\theta(\bar{2}01)$	a	-0.4420	$+17.868$	17	.0049
	Triclinic Or<40	$2\theta(\bar{2}01)$	a	$-.3982$	$+16.921$	12	.0057
	Monoclinic Or≥40	$2\theta(060)$	b	$-.2996$	$+25.478$	17	.0031
	Triclinic Or<40	$2\theta(060)$	b	$-.2194$	$+22.127$	12	.0034 (2−0.0027)
	Monoclinic Or≥40	$2\theta(\bar{2}04)$	c	$-.1373$	$+14.159$	17	.0014
	Triclinic Or<40	$2\theta(\bar{2}04)$	c	$-.0987$	$+12.189$	8	.0010
P50-56KF (Orthoclase) Wright and Stewart, (1968)	Monoclinic Or≥40	$2\theta(\bar{2}01)$	a	$-.4408$	$+17.838$	8	.0040
	Triclinic Or<40	$2\theta(\bar{2}01)$	a	$-.4262$	$+17.527$	3	.0009
	Monoclinic Or≥40	$2\theta(060)$	b	$-.2782$	$+24.585$	8	.0019
	Triclinic Or<40	$2\theta(060)$	b	$-.1599$	$+19.624$	3	.0067

TABLE 5—(*continued*)

Feldspar series	Symmetry and Composition	Variables		Equation, $y = mx + b$		No. of Observations	Standard error of y[a]
		x	y	m	b		
	Monoclinic Or≥40	$2\theta(\overline{2}04)$	c	−.1296	+13.897	8	.0017
	Triclinic Or<40	$2\theta(\overline{2}04)$	c	−.1088	+12.710	3	.0012
	Triclinic Or≥40	$2\theta(\overline{2}01)$	a	−.4367	+17.756	7	.0022
	Triclinic Or<40	$2\theta(\overline{2}01)$	a	−.3841	+16.613	4	.0025
Maximum microcline–low albite Orville (1967)	Triclinic Or≥40	$2\theta(060)$	b	−.2967	+25.367	7	.0013
	Triclinic Or<40	$2\theta(060)$	b	−.2556	+23.644	3	.0015
	Triclinic Or≥40	$2\theta(\overline{2}04)$	c	−.1271	+13.644	7	.0011 (3−.0010)
	Triclinic Or<40	$2\theta(\overline{2}04)$	c	−.1011	+12.324	4	.0046

[a] Where the best fit is not linear the degree and standard error of the best fit equation are given in parenthesis, *e.g.* (2−0.0041) for a quadratic equation with a standard error of 0.0041 in y.

Part I (Table 9 and discussion following) are also used here as examples of the method. The 2θ values for $\bar{2}01$, 060, and $\bar{2}04$ are as follows:

Specimen	$2\theta(\bar{2}01)$	$2\theta(060)$	$2\theta(\bar{2}04)$
X	21.180	41.610	50.840
Y	21.026	41.741	50.675
Z	20.940	41.891	50.775

These feldspars can be described as follows:

1. Specimen X is a sanidine having a structural state between that of high sanidine and *Puye* equivalents. Composition estimated from $\bar{2}01$ is Or$_{76}$.

2. Specimen Y is slightly anomalous and has an approximate structural state intermediate to equivalents of SH-1070 and Spencer B.

3. Specimen Z is highly anomalous; $\bar{2}01$ (derived from Fig. 3)—$\bar{2}01$ (observed) $= 0.6°$ 2θ. Apparent structural state is close to that of Spencer B. Composition cannot be estimated.

TABLE 6. EQUATIONS RELATING CELL DIMENSIONS TO OBSERVED 2θ VALUES OF SINGLE DIFFRACTION PEAKS FOR POTASSIUM-RICH ALKALI FELDSPARS

Type of Feldspar	Variables		Equation, $y = mx + b$		No. of Observations	Standard error of y[a]
	x	y	m	b		
Monoclinic	$2\theta(\bar{2}01)$	a	$-.4389$	$+17.799$	40	.0039
	$2\theta(060)$	b	$-.2908$	$+25.111$	40	.0022
	$2\theta(\bar{2}04)$	c	$-.1278$	$+13.678$	39	.0011
Maximum microcline	$2\theta(\bar{2}01)$	a	$-.2790$	$+14.440$	10	.0048 (2−.0046)
	$2\theta(060)$	b	$-.2687$	$+24.195$	7	.0014
	$2\theta(\bar{2}04)$	c	$-.1196$	$+13.262$	10	.0011

	$2\theta(\bar{2}01)$	a	$2\theta(060)$	b	$2\theta(\bar{2}04)$	c	$2\theta(131)$-$2\theta(1\bar{3}1)$
Intermediate microcline	21.053	8.5644	41.745	12.9705	50.615	7.2077	0.293
	21.045	8.5638	41.718	12.9793	50.688	7.1993	0.215
	21.025	8.5770	41.788	12.9628	50.778	7.1897	0.105
	20.998	8.5784	41.792	12.9569	50.583	7.2128	0.240

[a] See footnote, Table 5.

These descriptions do not differ significantly from those given in Part I (p. 71) using the axial cell dimensions a, b, and c.

The 'three-peak' method outlined is sufficient, so far as is known, to enable the identification and description of alkali feldspars encountered routinely in petrologic studies. In studies aimed specifically at identifying variations in the properties of a related group of alkali feldspars it is desirable to compute the unit-cell dimensions more precisely from fully measured X-ray diffraction patterns. For this purpose, the equations given in Tables 5–7 may be used to yield starting parameters for a cell refinement.

The standard errors associated with a, b, and c for the equations relating reflection-position to axial dimension are very close to the average

TABLE 7. EQUATIONS RELATING CELL DIMENSIONS TO CALCULATED 2θ VALUES OF SINGLE DIFFRACTION PEAKS FOR NATURAL ANORTHOCLASES

Variables		Equation, $y = mx + b$		No. of Observa- tions	Standard error of y
x	y	m	b		
$2\theta(\bar{2}01)$	a	$-.4046$	$+17.058$	21	.0008
$2\theta(060)$	b	$-.2311$	$+22.622$	21	.0010
$2\theta(\bar{2}04)$	c	$-.1060$	$+12.567$	21	.0005

standard error associated with the respective dimensions computed in a complete refinement of the unit cell; *i.e.* 1 part in 2500 for a, 1 part in 6000 for b, and 1 part in 6000 for c. This is not to say that the 'three-peak' method is a substitute for a good computer refinement, but does indicate that in most cases the determination of the composition and structural state of a feldspar and identification of whether or not a feldspar is anomalous using the 'three-peak' method will agree with that obtained from the methods given in Part I using the cell parameters. In natural suites of alkali feldspars studied by the author (Wright and Stewart, unpublished data) there are no significant differences in interpretation using the two methods.

APPENDIX: EQUATIONS RELATING CELL DIMENSION AND OBSERVED 2θ
VALUES FOR SINGLE DIFFRACTION PEAKS

Alkali feldspar series of constant structural state. Equations relating 2θ
values ($CuK\alpha_1$ measured according to the procedure described in Part I,
Appendix) to axial dimension are given in Table 5 for three complete
series of alkali feldspars described previously (Wright and Stewart,
1968; Orville, 1967). For each series the 2θ value and computed axial
dimension are related in two linear segments intersecting at a composi-
tion of $Or_{40}Ab_{60}$. In the series structurally equivalent to *high sanidine*
and to P50-56F orthoclase this intersection is coincident with the com-
position at which the symmetry changes from monoclinic to triclinic. An
intersection at the same composition was found for the maximum micro-
cline—low albite series although all members of this series are triclinic.[1]
Thus in each series the data for compositions more potassic than Or_{40}
were treated separately from data for compositions more sodic than
Or_{40}. For each set of data consisting of more than 5 points, 3rd, 2nd, and
1st degree polynomials were computed using a least-squares program. If
the data set contained 5 or less points only a linear fit was computed; in
larger data sets the differences in standard error for higher order equa-
tions were so small that a linear relationship was assumed. These equa-
tions can be used to obtain starting parameters for refinement of the cell
dimensions of any homogeneous alkali feldspar of essentially binary com-
position ($Or+Ab>95\%$), but, for reasons given below, are not applic-
able either to alkali feldspar phases in perthites or to alkali feldspars of
ternary composition.

Natural potassium-rich alkali feldspars. Equations relating observed 2θ
value to axial dimension were computed from data for 40 monoclinic
potassium-rich alkali feldspars, and 10 maximum microclines. These
equations are listed in Table 6 along with 2θ's and axial dimensions for
4 intermediate microclines. The data used to derive those equations are
mostly obtained from refinement of the cell dimensions of perthitic
orthoclases. Plots of 2θ values against cell dimension for perthitic ortho-
clases were made and it was found that additional potassium-rich alkali
feldspars, including one cryptoperthitic high sanidine, three feldspars
with anomalous cell dimensions, possibly low sanidine, and four homog-
eneous potassic feldspars (Or_{90}), fit the lines constructed for perthitic
orthoclases. Taken together, the natural monoclinic potassium-rich

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[1] A change of slope was previously suggested by examination of the variation of cell
dimensions with *Or* content across the maximum microcline-low albite series. (See Part I).

feldspars show a very limited range for a (8.48–8.62 Å) but have wide variations in b and c which can be related to the structural state and whether or not the cell dimensions are anomalous. The natural mono-clinic feldspars are thus distinguished from the feldspars of the synthetic high-sanidine series and alkali-exchanged orthoclase series for which a, b, and c all vary together with changing composition. The equations of Table 6 must be used to derive starting cell parameters for perthitic potassium-rich feldspars. The starting parameters for homogeneous monoclinic potassium-rich feldspars may be derived either from the equations of Table 6 or, if the structural state is known to be orthoclase or high sanidine, the appropriate equations of Table 1.

Although separate equations have been computed in Table 6 for monoclinic potassium-rich feldspars and for maximum microclines, only the equation relating 2θ (060) to b differs significantly between the two sets of data. Starting parameters for intermediate microclines must be obtained by interpolation of the values given from the equations for monoclinic potassium-rich feldspars and for maximum microclines.

Natural sodium-rich and ternary feldspars. The unit-cell dimensions of anorthoclases described by Carmichael and Mackenzie (1964) have been used to calculate 2θ values for $\overline{2}01$, 060, and $\overline{2}04$. The unit-cell dimensions of six anorthoclases refined by D. B. Stewart (unpub. data) have been included with these and equations relating the calculated[1] reflection positions and cell dimensions of the anorthoclases are given in Table7. On the assumption that all natural anorthoclases are comparable to those studied by Carmichael and Mackenzie (1964) and by Stewart the starting parameters for refinement of natural anorthoclases are best de-rived from the equations of Table 7.

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[1] Because observed values of 2θ were not published by Carmichael and Mackenzie (1964), calculated values of 2θ were used. As noted previously, this introduces a small bias when observed 2θ's of natural anorthoclases are used to calculate dimensions from the equations of Table 7.

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