

CALCULATED POWDER PATTERNS. PART II. SIX
POTASSIUM FELDSPARS AND BARIUM
FELDSPAR¹

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ABSTRACT

Integrated (I_{INT}) and peak (I_{PK}) intensities are calculated from single-crystal structure analyses for maximum microcline (granitic and authigenic), intermediate microcline, orthoclase, adularia, high sanidine and celsian. Graphical representation of the intensities distributed over Cauchy profiles results in plots which are very similar to comparable experimental X-ray diffraction traces over the whole 2θ range. Apparent differences in peak heights in the calculated and experimental patterns can be related to preferred orientations of crystals in standard mounts because of cleavage production during grinding.

INTRODUCTION

Among the rock-forming minerals, the ubiquitous feldspars are most important as indicators of the thermal history of a rock. Accurate determination of the chemical composition, cell size and crystal structure of the feldspar is of some use in categorizing the mineral as to its temperature of formation.

Both single-crystal patterns and powder patterns can be used to obtain the necessary information. Powder patterns are more readily obtainable but suffer from problems of preferred orientation, coincidence and overlap of reflections, and the difficulty of obtaining a single-phase sample. Preferred orientation can be minimized by careful sample preparation. Overlap can be compensated for by creating a complete set of standard powder patterns which can then be used to define the sensitive regions and distinguishing criteria for particular species. This set of standards may be either experimental or calculated from known crystal structure determinations. As accurate structure determinations of the calculated standard increases because it yields an "ideal" pattern free of the defects inherent in the experimental ones.

Part I (Borg and Smith, 1968) of this series presented the calculated X-ray powder patterns for five members of the plagioclases. This paper contains comparable data for potassium and barium feldspars. These patterns are shown to compare very well with experimental patterns and serve as a guide to the indexing and interpretation of the experimental patterns.

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SOURCE OF DATA FOR CALCULATIONS

Computations are based on data from seven published structure analyses all based on three-dimensional intensity data having R factors in range from 0.054 to 0.138. The six potassium feldspars for which powder patterns have been calculated include maximum microcline (igneous) (Brown and Bailey, 1964), maximum microcline (authigenic) (Finney and Bailey, 1964), intermediate microcline (Bailey and Taylor, 1955), orthoclase (Colville and Ribbe, 1968), sanidine (heat-treated orthoclase) (Ribbe, 1963), and adularia (Colville and Ribbe, 1968). The barium feldspar (celsian) structure was determined by Newnham and Megaw (1960). All of the potassium feldspars closely approach the composition of the end member KAlSi_3O_8 (Table 1).

Minor Na, Ca and Ba were generally ignored in the structure refinements, and small amounts of co-existing Na-feldspar in the micropertites did not interfere with the structure analyses (Bailey and Taylor, 1955; p. 622). Accordingly, their effects were also omitted in the computations presented here. As far as possible, the exact site occupancies (or weighted scattering factors) and temperature factors were used in the computations, as were reported in the structure investigations. The temperature factors thus compensate for the small contribution of minor constituents. If the state of ionization of the atomic scattering factors used was not given, a fully ionized state was assumed. When available, anisotropic temperature factors were used for the large cations (K, Ba) and isotropic for the remaining ions. The Si/Al distribution summarized in Table 1 derives from a consideration of the size of the tetrahedra. In some cases, they differ slightly from those given in the original publications because the relationship between T-O distance and Al content has been subject to review (Smith and Bailey, 1963; Ribbe and Gibbs, 1967; Stewart and Ribbe, 1967). There is some indication that approximations of Al-content are only accurate to ± 8 percent, and Appleman and Clark (1965) question the evidence for partial disorder in maximum microcline.

Calculations for both orthoclase and adularia are based on $C2/m$ symmetry although the presence of weak, diffuse reflections $h+k=\text{odd}$ indicate a lower symmetry ($P2_1/a$) for the unit cell (Laves and Goldsmith, 1961; Colville and Ribbe, 1968). These reflections, which were ignored in the original structural study, probably have no expression in experimental powder patterns. Similarly, the triclinic domains described most recently by McConnell (1965), Gubser and Laves (1967), and Colville and Ribbe (1968) have not been taken into account because the average structures are monoclinic.

POWDER PATTERN CALCULATIONS

The powder patterns listed in Tables 2-8 and shown in Figures 1-6 were calculated using the POWD2 and XCHART programs described by Smith (1967). An evaluation of the use of these programs to simulate complicated patterns has been given by Smith (1968), and its specific application to feldspar patterns was discussed by Borg and Smith (1968). For completeness of the present paper, a summary of the more important characteristics follows:

Integrated intensities and their associated d -values are calculated directly from the crystal structure. This integrated intensity is assumed to be distributed over a Cauchy-shaped diffraction maximum. The width of the peak at half-maximum is a function of the diffraction angle, 2θ , and the values used were based on empirically determined relationships

TABLE 1. DESCRIPTION OF FELDSPARS

Variety	Max. Microcline (granitic)	Max. Microcline (autohgenic)	Intermediate Microcline	Adularia	Orthoclase	High Sanidine (heated orthoclase)	Celsian
Composition (Mol %)	$\sim\text{Or}_{98}\text{Ab}_2$ (within a perthite, $\text{Or}_{94}\text{Ab}_6\text{An}_0$)	Or_{100}	$\sim\text{Or}_{100}$ (within a microper- thite, $\text{Or}_{85}\text{Ab}_{15}\text{An}_{0}$)	$\text{Or}_{95}\text{Ab}_5$ Cs	$\text{Or}_{100}\text{Ab}_0$ An	$\text{Or}_{90}\text{Ab}_{10}$ An	$\text{Ba}_{0.81}\text{K}_{0.18}$ $\text{Al}_{1.99}\text{Si}_{2.01}\text{O}_8$
Source	Peltooslo, Russia Helsinki #SM4709	Pontiskalk limestone, Switzerland	Kodarma, Bihar India (Spencer U)	St. Gotthard, Swit- zerland (Spencer B)	Mogok, Upper Bur- ma (Spencer C)	Mogok, Upper Bur- ma (Spencer C)	Broken Hill, N.S.W.
<i>a</i> (Å)	8.560	8.5726	8.5784	8.554	8.561	8.5642	8.627
<i>b</i>	12.964	12.9618	12.9600	12.970	12.996	13.0300	13.045
<i>c</i>	7.215	7.2188	7.2112	7.207	7.192	7.1749	14.408
α	90° 39'	90° 34'	89° 42'				
β	115° 50'	115° 55'	115° 58'	116° 0.4'	116° 0.6'	115° 59'	115° 13'
γ	87° 42'	87° 45'	90° 52.5'				
Space group	CI	CI	CI	$C2/m(P2_1/a)$	$C2/m(P2_1/a)$	$C2/m$	$I2/c$
Site occupancy (% Si)							
T ₁ (o)	6 ^a	10 ^a	31 ^a	61	65	75 ^a	B ₁ (0)70 ^b
T ₁ (m)	97	97	73	61	65	75	B ₁ (2)23
T ₂ (o)	99	93	97	89	85	75	B ₂ (0)27
T ₂ (m)	98	100	99	89	85	75	B ₂ (2)82
R	0.104	0.085	0.138	0.055	0.054	0.099	0.069
Reference	Brown & Bailey (1964)	Finney & Bailey (1964)	Bailey & Taylor (1955)	Colville & Ribbe (1968)	Colville & Ribbe (1968); Jones & Tay- lor (1961)	Ribbe (1963); Cole, Newnham & Megaw et al. (1949)	(1960)
ASF	0.0454	0.0452	0.0539	0.0575	0.0574	0.0561	0.161

^a Brown & Bailey (1964) based on 1.00 Al.^b Taylor (1962, p. 15).

TABLE 2. CALCULATED POWDER DATA FOR MAXIMUM MICROCLINE (GRANITIC)—CuK α .

2 θ (hkl)	2 θ (PK)	d	hkl	I(INT)	I(PK)	2 θ (hkl)	2 θ (PK)	d	hkl	I(INT)	I(PK)
13.13	13.14	6.736	110	6	5	49.90	49.92	1.826	262	2	2
13.62	13.66	6.494	001	3	5	49.92		1.825	420	2	
13.66		6.477	020	4		50.49		1.806	043	5	
14.94	14.95	5.923	111	6	4	50.55		1.804	062	6	
15.26	15.28	5.800	111	4	7	50.56	50.56	1.804	441	4	10
19.26	19.28	4.603	021	4	3	50.57		1.803	204	29	
21.07	21.08	4.213	201	76	51	50.75		1.797	442	2	0
22.20	22.30	3.984	111	17	12	50.88		1.793	043	8	
22.64	22.66	3.924	111	8	6	50.93		1.791	062	8	9
23.09	23.20	3.849	200	7	0	51.03	50.90	1.788	350	2	
23.20		3.831	130	44	30	51.18		1.783	262	4	0
24.00	24.02	3.704	130	46	30	51.63	51.64	1.769	242	3	2
24.35	24.36	3.652	131	15	11	52.63		1.738	441	4	
24.74	24.76	3.595	221	13	0	52.74	52.68	1.734	114	2	3
24.95	24.94	3.566	131	6	0	52.97		1.727	242	2	0
25.55	25.56	3.484	112	40	29	54.07	54.08	1.694	353	3	2
25.64		3.471	221	2		55.39	55.40	1.658	351	5	3
25.88	25.66	3.466	112	29	26	55.54		1.653	172	3	4
26.44	26.44	3.368	220	67	41	55.59		1.652	353	5	
27.11	27.12	3.286	202	73	46	56.03	56.02	1.640	172	2	1
27.39	27.46	3.253	220	62	100	56.81	56.80	1.619	080	3	2
27.45		3.247	002	100		56.95	56.94	1.616	513	2	2
27.52		3.238	040	42		57.46	57.48	1.602	424	4	4
29.43	29.44	3.033	131	33	10	57.48		1.602	351	5	
30.15	30.24	2.961	222	6	26	58.24	58.26	1.583	424	4	3
30.23		2.954	131	15		58.45	58.44	1.578	024	4	3
30.68		2.912	022	8		58.68	58.68	1.572	024	5	3
30.73	30.74	2.907	041	19	17	58.83	58.82	1.568	081	2	2
30.90		2.900	222	3		59.39	59.40	1.555	223	2	1
30.87		2.894	022	6	0	59.67	59.68	1.548	533	6	3
30.93	30.92	2.889	041	13	13	59.94	59.94	1.542	481	6	3
32.15	32.16	2.782	132	11	7	61.16	61.16	1.514	280	16	7
32.43	32.48	2.758	311	2	10	61.27		1.512	533	4	
32.47		2.755	132	16		62.71	62.72	1.480	461	5	3
34.24		2.616	312	9		63.11	63.12	1.472	280	13	7
34.24	34.26	2.616	241	21	17	63.13		1.472	514	4	
34.28		2.614	221	1		63.26	63.28	1.469	530	2	6
34.72	34.74	2.581	312	13	8	63.78		1.458	114	5	
34.88	34.82	2.570	112	8	8	63.88	63.96	1.456	173	2	7
35.12	35.14	2.553	221	3	0	63.92		1.455	243	7	
35.15		2.551	112	3		63.98		1.454	463	2	
35.36	35.38	2.536	310	5	0	65.05	65.22	1.432	530	2	4
35.46	35.58	2.528	240	2	15	65.21		1.429	243	5	
35.56		2.521	241	26		65.49	65.48	1.424	602	10	5
35.91	35.92	2.489	310	6	4	66.32	66.32	1.408	402	9	5
36.93	36.96	2.432	151	7	6	66.50	66.50	1.405	190	2	4
36.94		2.431	240	3		67.05	67.06	1.395	405	4	3
37.07	37.06	2.423	331	11	8	67.25	67.24	1.391	264	3	2
37.62	37.62	2.389	151	4	2	68.47	68.48	1.369	425	3	2
38.53		2.334	331	6		69.04	69.04	1.359	621	3	2
38.56	38.60	2.333	113	4	7	70.09	70.10	1.341	192	3	1
38.61		2.330	113	6		70.65	70.64	1.332	192	4	2
39.21	39.22	2.296	332	3	3	71.01	71.00	1.326	604	4	2
40.49	40.52	2.226	332	2	2	71.53	71.58	1.318	135	3	3
40.52		2.224	151	2		71.59		1.317	135	5	
41.53		2.172	151	3	0	72.15	72.16	1.308	482	5	4
41.79	41.80	2.160	241	12	21	72.29	72.32	1.306	204	4	4
41.81		2.159	060	31		72.40		1.304	515	2	
42.75	42.78	2.113	401	5	3	73.11	73.14	1.293	282	7	4
42.90	42.88	2.106	402	7	5	73.52		1.287	441	2	0
43.21	43.20	2.092	241	5	3	73.74	73.76	1.284	392	2	3
43.48	43.58	2.079	311	2	3	73.76		1.283	600	3	
43.56		2.076	202	3		74.57	74.58	1.271	445	3	2
43.98	44.06	2.057	311	2	11	74.91	75.00	1.267	535	3	3
44.06		2.053	061	3		75.02		1.265	355	3	
44.28	44.28	2.044	051	5	1	75.31	75.32	1.261	282	8	6
44.69	44.70	2.026	422	6	3	75.32	75.32	1.261	482	9	5
45.49	45.50	1.992	222	9	5	80.18	80.26	1.196	316	3	2
45.76	45.76	1.981	422	13	7	80.30		1.195	2102	2	
45.93	45.88	1.974	333	3	5	81.13	81.12	1.184	733	2	1
46.23	46.24	1.962	222	7	4	82.48	82.50	1.168	484	3	1
46.36	46.36	1.956	351	3	4	84.02	84.04	1.151	084	3	2
47.18	47.18	1.925	400	16	8	84.46	84.46	1.146	516	2	2
47.58	47.58	1.910	403	9	5	84.82	84.82	1.142	084	3	2
48.04	48.04	1.892	261	2	1	85.14		1.139	484	3	2
48.76	48.78	1.866	113	6	4	85.25	85.16	1.138	443	3	
48.92	48.94	1.860	350	3	5	86.97	86.96	1.119	733	2	1
48.99	48.98	1.858	152	2	5	87.28	87.26	1.116	443	3	1
49.00		1.857	113	4		90.36		1.086	733	2	0
49.15	49.12	1.852	260	3	4	90.79	90.80	1.082	135	3	2

TABLE 3. CALCULATED POWDER DATA FOR MAXIMUM MICROCLINE (AUTHENTIC)—CuK α .

2 θ (hkl)	hkl (PK)	d	hkl	I(NT)	(PK)	2 θ (hkl)	hkl (PK)	d	hkl	I(NT)	(PK)
13.13	13,14	6.738	110	6	3	49.00		1.857	132	2	
13.59		6.511	110	1		49.02		1.857	113	4	5
13.63	13,66	6.493	001	3	6	49.13		1.853	260	3	
13.66		6.476	020	4		49.87	49.80	1.827	420	2	2
14.84	14,94	5.927	111	5	4	50.49		1.806	043	5	
15.24	15,26	5.808	111	4	3	50.53		1.805	411	4	
19.26	19,28	4.604	021	4	3	50.54	50.54	1.804	204	29	21
21.03	21,04	4.220	201	74	54	50.54		1.804	062	5	
22.30	22,30	3.983	111	17	12	50.71		1.799	442	2	6
22.65	22,66	3.923	111	7	6	50.90		1.793	043	7	
23.07	23,20	3.852	200	7	0	50.95	50.92	1.791	062	7	11
23.20		3.830	130	44	32	50.99		1.789	350	2	
24.00	24,00	3.705	130	44	31	51.14		1.784	262	4	0
24.35	24,36	3.652	131	14	11	51.64	51.64	1.769	242	3	3
24.73	24,74	3.597	221	12	9	52.56	52.58	1.740	441	4	3
24.93	24,92	3.569	131	7	6	52.73	52.72	1.734	114	2	3
25.54	25,56	3.485	112	37	30	52.98	52.98	1.727	242	2	3
25.60	25,66	3.477	221	2	30	54.06	54.06	1.695	353	3	2
25.66		3.468	112	31		55.40		1.657	351	5	
26.43	26,44	3.369	220	67	49	55.52	55.54	1.654	353	5	5
27.08	27,08	3.290	202	72	51	55.56		1.653	112	3	
27.37		3.256	220	62		56.01	56.00	1.640	112	2	1
27.45	27,46	3.246	002	100	100	56.82	56.82	1.619	080	3	3
27.52		3.238	040	38		57.40	57.44	1.604	424	4	4
29.43	29,44	3.032	131	32	20	57.46		1.602	351	5	3
30.13	30,24	2.963	222	6	29	58.15	58.16	1.585	424	4	2
30.23		2.954	131	41		58.46	58.46	1.577	024	4	2
30.68		2.912	022	7		58.70	58.70	1.571	024	5	3
30.73	30,74	2.907	041	19	18	59.60	59.60	1.550	533	6	3
30.76		2.904	222	3		59.93	59.92	1.542	461	6	3
30.89	30,92	2.893	022	7	14	61.15	61.18	1.514	533	4	11
30.93		2.888	041	13		61.18		1.514	280	16	
32.15	32,16	2.781	132	11	7	62.65	62.66	1.482	461	5	3
32.38		2.763	311	1	10	63.01	63.10	1.474	314	4	7
32.45	32,46	2.756	132	16		63.09		1.472	280	12	7
34.19		2.620	312	10		63.23	63.24	1.469	530	2	5
34.24	34,24	2.616	241	20	17	63.80		1.458	114	4	
34.28		2.614	221	11		63.86		1.456	113	2	
34.66	34,66	2.566	312	11	7	63.94	63.96	1.455	243	7	7
34.89	34,90	2.569	112	8	6	63.96		1.454	463	2	
35.12	35,16	2.553	221	3	5	64.99	65.02	1.434	530	2	2
35.16		2.550	112	4		65.23	65.24	1.429	243	5	4
35.33	35,34	2.538	310	5	5	65.38	65.38	1.426	602	9	5
35.49	35,34	2.527	240	2	15	66.31	66.32	1.408	402	9	5
35.54		2.524	241	25		66.50	66.50	1.405	190	2	4
35.88	35,88	2.501	310	5	4	66.98	66.98	1.396	405	4	2
36.92		2.433	240	3		67.26	67.16	1.391	264	2	2
36.94	37,04	2.431	151	7	9	68.41	68.40	1.370	425	3	2
37.05		2.424	331	11		68.96	68.96	1.361	621	2	2
37.60	37,60	2.390	151	4	3	70.12	70.12	1.341	132	3	2
38.48		2.338	331	5		70.63	70.64	1.332	192	4	2
38.55	38,56	2.333	113	4	7	70.88	70.86	1.328	504	4	2
38.60		2.331	113	6		71.52	71.60	1.310	135	3	3
39.18	39,18	2.297	332	3	2	71.60		1.317	135	4	3
40.42	40,52	2.230	332	2	2	72.14	72.16	1.308	462	5	4
40.53		2.224	151	2		72.28	72.30	1.306	515	2	4
41.54		2.172	151	3	0	72.31		1.306	204	4	
41.70	41,82	2.164	003	1	22	72.99	73.14	1.295	0100	2	4
41.79		2.160	241	12		73.13		1.293	282	6	
41.81		2.159	060	30		73.46		1.288	641	2	0
42.70	42,72	2.116	401	5	4	73.72	73.72	1.284	600	3	3
42.82	42,82	2.110	402	6	5	73.75		1.284	392	2	3
43.20	43,20	2.092	241	5	3	74.47	74.50	1.273	445	2	2
43.47	43,58	2.080	311	2	3	74.83	74.82	1.268	535	3	2
43.57		2.075	202	3		75.01	75.02	1.265	355	3	2
43.97	44,06	2.057	311	2	2	75.24	75.26	1.262	462	8	5
44.06		2.053	061	3		75.32		1.261	282	7	2
44.29	44,30	2.043	051	5	3	80.13	80.14	1.197	316	3	2
44.63	44,64	2.028	222	6	4	80.27	80.24	1.195	2102	2	2
45.51	45,52	1.892	222	9	5	81.01	81.02	1.188	733	2	1
45.68	45,68	1.884	322	12	6	82.47	82.46	1.169	484	3	2
45.90		1.876	333	3	0	84.02	84.02	1.151	084	3	2
46.24	46,24	1.862	222	7	4	84.34	84.30	1.147	516	2	2
46.37	46,36	1.857	351	3	4	84.86		1.142	084	3	2
47.14	47,14	1.826	400	15	8	85.04	85.06	1.140	464	3	2
47.50	47,50	1.813	403	9	6	85.27	85.24	1.137	443	3	2
48.01	48,02	1.893	261	2	1	86.87	86.86	1.120	753	2	1
48.35	48,36	1.881	351	2	1	87.29	87.28	1.116	433	2	1
48.78	48,78	1.865	113	6	4	90.18	90.22	1.088	753	2	1
48.92	48,92	1.860	350	3	5	90.83	90.82	1.081	155	3	2

TABLE 4. CALCULATED POWDER DATA FOR INTERMEDIATE MICROCLINE—CuK α

2 θ (hkl)	2 θ (PK)	d	hkl	I(INT)	I(PK)	2 θ (hkl)	2 θ (PK)	d	hkl	I(INT)	I(PK)
13.26	13.28	6.669	110	5	4	43.60	43.62	2.074	202	3	4
13.43	13.44	6.585	110	2	2	43.63		2.073	311	2	
13.65	13.66	6.483	001	2	6	43.80	43.72	2.065	311	3	3
13.65		6.479	020	4		44.14	44.16	2.050	061	3	4
15.02	15.04	5.893	111	5	5	44.18		2.048	061	4	
15.15	15.16	5.842	111	5	5	44.90	44.90	2.017	222	7	4
19.34	19.36	4.587	021	3	3	45.31	45.32	2.000	222	10	5
21.01	21.02	4.225	201	74	58	45.78	45.78	1.980	222	8	5
22.43	22.44	3.961	111	13	11	46.03	46.02	1.970	222	7	5
22.55		3.940	111	9		46.17	46.16	1.964	333	3	4
23.05	23.06	3.856	200	8	7	46.60	46.60	1.947	333	2	2
23.44	23.44	3.792	130	46	36	46.94	47.10	1.934	351	2	0
23.73	23.74	3.746	130	47	37	47.10		1.928	400	12	7
24.51	24.52	3.629	131	14	12	47.46	47.48	1.914	403	7	5
24.75	24.76	3.593	131	9	8	48.93	49.00	1.860	113	4	4
24.97	24.98	3.563	221	10	9	49.00		1.857	113	4	
25.31	25.34	3.515	221	5	7	49.38	49.52	1.844	152	2	3
25.59	25.66	3.477	112	41	47	49.54	49.52	1.838	350	2	3
25.66		3.468	112	34		50.24		1.814	262	2	0
26.71	26.72	3.335	220	70	53	50.31	50.62	1.812	350	2	0
27.06	27.08	3.293	220	67	100	50.60		1.802	204	23	15
27.08		3.290	202	73		50.70		1.799	043	5	
27.49	27.50	3.242	002	100	96	50.71		1.799	062	4	5
27.51		3.240	040	35		50.77	50.74	1.797	262	2	
29.70	29.72	3.005	131	37	26	50.78		1.796	043	6	
29.97	29.98	2.979	131	40	29	50.79		1.796	062	5	
30.31	30.32	2.946	222	5	5	51.10	51.10	1.786	441	4	3
30.58	30.84	2.921	222	3	0	51.88	51.88	1.761	441	3	2
30.80		2.901	022	6	52.11	52.02	1.754	242	2	2	
30.81	2.900	041	17	27	54.47	54.46	1.683	353	3	2	
30.84	2.897	022	5	55.09	55.10	1.666	353	4	2		
30.85	2.896	041	15	55.65	55.66	1.650	172	3	2		
32.24	32.24	2.774	132	14	11	55.90	55.90	1.643	172	2	2
32.40	32.40	2.761	132	16	12	56.04	56.04	1.639	351	4	3
34.30	34.32	2.612	312	12	9	56.78	56.78	1.620	351	4	4
34.49	34.60	2.598	312	12	10	56.79		1.620	080	3	
34.55		2.593	221	2		57.61	57.62	1.599	424	4	2
34.61	2.589	241	22	57.93	57.94	1.590	424	3	2		
34.85	2.572	221	3	0	58.64	58.68	1.573	024	3	3	
35.02	2.560	112	7	58.69		1.572	024	4			
35.11	35.12	2.554	112	5	21	60.00	60.00	1.540	333	4	2
35.12		2.553	241	24		60.63	60.68	1.526	333	4	4
35.47	35.48	2.528	310	5	5	60.71		1.524	461	4	
35.68	35.68	2.514	310	6	5	61.74	61.74	1.501	280	10	6
35.92	2.498	240	1	0	61.75		1.501	461	4		
36.45	36.46	2.463	240	1	1	62.45	62.46	1.486	280	9	4
37.11	37.12	2.420	151	7	5	62.84	62.82	1.478	514	2	2
37.40	37.44	2.403	151	5	7	63.98	64.00	1.454	114	2	3
37.45		2.399	331	8		64.43	64.42	1.445	243	4	4
38.00	38.00	2.366	331	6	4	64.85	64.84	1.437	243	4	2
38.61	38.63	2.330	113	5	6	65.28	65.28	1.428	602	6	3
38.64		2.328	113	6		66.32	66.32	1.408	602	6	3
39.52	39.52	2.278	332	3	2	70.21	70.20	1.339	192	2	1
40.02	40.02	2.251	332	3	2	70.48	70.48	1.335	192	2	2
40.48	40.52	2.227	132	1	2	70.81	70.80	1.330	604	2	1
40.54		2.223	330	1		71.64	71.68	1.316	135	2	2
40.86	40.86	2.207	151	3	2	71.69		1.315	135	2	
41.08	41.20	2.195	330	1	3	72.41	72.40	1.304	204	2	1
41.20		2.189	151	3		73.02	73.00	1.295	362	3	2
41.79	41.80	2.150	060	28	16	73.85	73.86	1.282	282	3	2
42.25	42.26	2.137	241	8	5	74.24	74.22	1.276	482	4	3
42.64	42.74	2.119	401	6	9	74.59	74.58	1.271	282	4	3
42.74		2.114	241	5							
42.77	2.112	402	6								

TABLE 5. CALCULATED POWDER DATA FOR ADULARIA—CuK α .

2 θ (hkl)	2 θ (PK)	d	hkl	I(INT)	I(PK)	2 θ (hkl)	2 θ (PK)	d	hkl	I(INT)	I(PK)
13.38	13.38	6.613	110	5	6	54.80	54.80	1.674	353	6	4
13.64	13.66	6.485	020	4	6	55.74	55.74	1.648	372	4	3
13.66		6.477	001	2		56.35	56.50	1.631	334	1	5
15.10	15.10	5.863	111	7	8	56.50		56.50	1.627	351	
19.35	19.36	4.583	021	2	3	56.64	56.64	1.624	313	1	5
21.06	21.06	4.215	201	59	61	56.73		1.621	080	2	
22.53	22.54	3.943	111	18	19	57.83	57.84	1.593	324	6	4
23.12	23.12	3.844	200	5	6	58.72	58.72	1.571	024	6	5
23.59	23.60	3.768	130	72	72	59.23	59.24	1.559	223	1	1
24.62	24.64	3.612	131	15	15	60.43	60.44	1.531	533	8	5
25.18	25.18	3.534	221	10	11	60.56	60.58	1.528	063	2	5
25.64	25.64	3.471	112	52	50	61.30	61.30	1.511	361	8	5
26.94	26.94	3.307	220	100	100	62.08	62.08	1.494	280	22	14
27.11	27.10	3.286	202	60	75	62.84	62.84	1.478	514	4	3
27.48	27.52	3.243	040	30	100	63.74	63.74	1.459	173	3	2
27.52		3.239	002	78		64.10	64.24	1.451	114	4	5
29.86	29.86	2.990	131	57	51	64.24		64.24	1.449	530	
30.47	30.48	2.932	222	8	8	64.73	64.74	1.439	243	9	6
30.81	30.82	2.899	041	25	31	64.86	64.88	1.436	460	2	5
30.83		2.897	022	10		65.10	65.06	1.432	363	2	3
32.15		2.782	311	1	0	65.32	65.32	1.427	552	2	4
32.32	32.32	2.768	132	22	19	65.49	65.48	1.424	602	7	5
34.46	34.46	2.600	312	18	15	65.88	65.88	1.416	190	2	2
34.77	34.88	2.578	221	4	33	66.52	66.52	1.404	402	7	4
34.88		2.570	241	37		67.07	67.06	1.394	305	3	2
35.12	35.10	2.553	112	8	10	67.63		1.384	553	2	
35.68	35.68	2.514	310	8	7	67.64	67.64	1.384	264	4	5
36.21	36.22	2.478	240	3	3	67.65		1.384	134	2	
37.23	37.24	2.413	151	9	7	68.81	68.82	1.363	425	2	1
37.79	37.80	2.378	531	12	9	69.75	69.76	1.347	621	2	2
38.65	38.66	2.328	113	7	6	70.29	70.30	1.338	192	6	4
39.82	39.82	2.262	332	3	3	70.96	70.96	1.327	804	2	2
40.33	40.36	2.234	223	1	1	71.71	71.72	1.315	135	6	4
40.40		2.231	132	1		72.02	71.92	1.310	345	2	3
40.90	41.02	2.204	330	1	4	72.16	72.16	1.308	515	2	2
41.03		2.198	151	5		72.43	72.44	1.304	531	2	3
41.75	41.76	2.162	060	25	19	72.54	72.54	1.302	204	3	3
41.80		2.159	003	1		72.86	72.90	1.297	0100	2	3
42.54	42.54	2.123	241	11	9	72.90		1.296	083	2	
42.77	42.78	2.112	401	3	5	73.66	73.66	1.285	482	11	7
42.88	42.88	2.107	402	5	6	73.90	73.88	1.281	600	2	6
43.57		2.076	133	1	0	73.93		1.281	445	3	
43.70	43.70	2.070	202	2	3	74.24	74.24	1.276	282	11	7
43.84	43.84	2.063	311	3	3	74.84	74.86	1.268	641	3	3
44.13	44.14	2.050	061	5	4	74.92		1.266	392	2	
45.20	45.20	2.004	422	14	10	75.52	75.52	1.258	535	3	4
45.89	46.00	1.972	222	12	9	75.56		1.257	355	4	
46.42	46.42	1.954	333	3	3	79.35	79.36	1.206	2102	2	2
47.25	47.26	1.922	400	11	9	80.20	80.22	1.196	316	3	2
47.36	47.36	1.918	351	3	9	82.12	82.12	1.173	733	2	1
47.55	47.54	1.911	403	6	6	83.73	83.74	1.154	484	4	2
48.26	48.30	1.884	260	3	3	84.27	84.50	1.148	516	2	3
48.33		1.882	331	2		84.49		1.146	084	5	
49.03	49.04	1.856	113	7	6	86.52	86.52	1.124	443	3	1
49.42	49.42	1.843	420	2	3	87.73	87.72	1.112	194	2	1
49.56	49.56	1.838	152	2	3	88.61	88.64	1.103	753	3	2
49.70	49.68	1.833	423	1	3	89.47	89.44	1.094	710	2	1
49.99	49.98	1.823	350	4	3	90.46	90.46	1.085	155	3	1
50.49	50.64	1.806	262	5	0	93.01	93.02	1.062	683	2	1
50.63		1.801	204	23		22	93.26	93.28	1.060	565	2
50.73	50.74	1.798	062	10	24	94.07	94.14	1.053	2104	2	1
50.76		1.797	043	10		94.20		1.051	590	2	
51.59	51.60	1.770	441	7	6	109.43	109.46	0.944	557	2	1
51.69		1.767	442	3		113.21		0.923	396	2	0
52.40	52.40	1.745	242	4	3	114.99	115.02	0.913	794	2	1
53.19	53.18	1.721	133	2	1	117.68	117.66	0.900	596	2	1
54.06	54.08	1.695	512	2	1	118.42	118.06	0.897	2123	2	1

TABLE 6. CALCULATED POWDER DATA FOR ORTHOCLASE—CuK α .

2 θ (hkl)	2 θ (PK)	d	hkl	I(INT)	I(PK)	2 θ (hkl)	2 θ (PK)	d	hkl	I(INT)	I(PK)
13.36	13.38	6.621	110	5	6	54.02	54.02	1.696	512	2	2
13.62	13.62	6.498	020	5	7	54.78	54.78	1.674	353	6	4
13.69		6.464	001	2		55.67	55.68	1.650	172	4	3
15.10	15.12	5.861	111	6	7	56.42	56.44	1.629	334	1	6
19.35	19.36	4.583	021	2	3	56.44		1.629	351	7	
21.05	21.06	4.217	201	57	61	56.61	56.60	1.625	080	2	5
22.54	22.54	3.941	111	17	18	56.62		1.624	513	1	
23.10	23.12	3.847	200	5	6	57.89	57.90	1.592	424	6	4
23.55	23.56	3.775	130	74	75	58.84	58.84	1.568	024	6	5
24.60	24.60	3.616	131	15	16	59.30	59.30	1.557	223	2	2
25.15	25.15	3.537	221	10	11	60.40	60.40	1.531	533	8	6
25.69	25.69	3.465	112	52	51	60.56	60.56	1.528	063	2	5
26.91	26.91	3.310	220	100	100	61.21	61.20	1.513	461	8	5
27.14	27.14	3.283	202	59	67	61.95	61.96	1.497	280	22	13
27.43	27.58	3.249	040	29	0	62.87	62.88	1.477	514	3	3
27.58		3.232	002	78	82	63.71	63.72	1.459	173	3	2
29.84	29.84	2.991	131	59	53	64.17	64.22	1.450	530	3	5
30.48	30.48	2.930	222	7	8	64.23		1.449	114	4	
30.77	30.78	2.903	041	25	25	64.76	64.78	1.438	460	2	7
30.87	30.84	2.894	022	11	24	64.77		1.438	243	9	
32.12		2.784	311	1	0	65.05	64.94	1.433	463	2	5
32.33	32.34	2.767	132	22	20	65.23	65.24	1.429	552	2	4
34.46	34.46	2.600	312	18	16	65.42	65.42	1.425	502	7	6
34.77	34.84	2.578	221	4	34	65.74	65.60	1.419	190	2	3
34.83		2.574	241	37		66.53	66.54	1.404	402	7	4
35.17	35.16	2.550	112	8	9	67.18	67.18	1.392	405	2	2
35.65	35.66	2.516	310	8	8	67.57	67.68	1.385	553	2	4
36.18	36.16	2.482	240	4	3	67.67		1.383	264	3	
37.17	37.18	2.417	151	9	7	67.75	67.75	1.382	134	2	
37.74	37.74	2.381	331	12	10	68.92	68.92	1.361	425	2	2
38.73	38.74	2.323	113	7	6	69.67	69.68	1.348	621	3	2
39.80	39.80	2.263	332	4	3	70.18	70.18	1.340	192	6	4
40.39	40.40	2.231	223	1	1	70.96	70.96	1.327	604	3	2
40.42		2.230	132	1		71.86	71.86	1.313	135	6	4
40.85	40.98	2.207	330	1	4	72.14	72.10	1.308	245	2	3
40.98		2.201	151	4		72.24		1.307	515	2	
41.66	41.66	2.166	060	25	19	72.38	72.36	1.304	531	2	3
41.89		2.155	003	1	0	72.66	72.66	1.300	204	3	3
42.51	42.52	2.125	241	11	9	72.70		1.300	0100	2	
42.73	42.72	2.114	401	4	6	72.86	72.88	1.297	083	2	3
42.85	42.84	2.108	402	5	6	73.53	73.54	1.287	482	10	7
43.62		2.073	133	1	0	73.84	73.74	1.282	600	2	5
43.74	43.84	2.068	202	2	4	74.02	74.16	1.280	445	3	7
43.83		2.064	311	3		74.16		1.277	282	10	
44.05	44.06	2.054	061	5	5	74.74	74.76	1.269	541	3	3
45.17	45.18	2.006	422	13	10	74.78		1.268	392	2	
46.02	46.02	1.970	222	12	9	75.60	75.62	1.257	535	3	4
46.44	46.44	1.954	333	3	3	75.65		1.256	355	4	
47.21	47.22	1.923	400	11	10	79.20	79.22	1.208	2102	2	2
47.29		1.920	351	3		80.40	80.42	1.193	316	3	3
47.56	47.56	1.910	403	6	5	82.04	82.04	1.174	733	2	1
48.17	48.18	1.887	260	2	2	83.68	83.68	1.155	484	4	2
48.30	48.30	1.883	331	2	3	84.42	84.48	1.146	516	2	3
49.12	49.12	1.853	113	7	6	84.49		1.146	084	4	
49.37		1.844	420	2	0	86.55	86.56	1.124	443	3	1
49.54	49.52	1.838	152	2	3	87.70	87.70	1.112	194	2	1
49.71	49.70	1.833	423	1	2	88.51	88.52	1.104	753	3	2
49.91	49.92	1.826	350	3	3	89.38	89.36	1.095	710	2	1
50.43	50.46	1.808	262	4	5	90.59	90.60	1.084	155	3	1
50.69		1.799	062	9		92.88	92.90	1.063	683	2	1
50.74	50.76	1.798	204	23	25	93.25	93.24	1.060	665	2	1
50.80		1.796	043	10		94.00	94.00	1.053	2104	2	2
51.52	51.54	1.772	441	7	6	94.02		1.053	590	2	2
51.63	51.64	1.769	442	3	5	109.63	109.62	0.942	557	2	1
52.40	52.40	1.745	242	4	3	114.82	114.80	0.914	794	2	1
53.25	53.26	1.719	133	2	1	117.70	117.78	0.900	596	2	1

TABLE 7. CALCULATED POWDER DATA FOR HIGH SANIDINE—CuK α .

2 θ (hkl)	2 θ (PK)	d	hkl	I(INT)	I(PK)	2 θ (hkl)	2 θ (PK)	d	hkl	I(INT)	I(PK)
13.35	13.36	6.628	110	5	6	50.63	50.64	1.801	062	8	8
13.58	13.58	6.515	020	6	8	50.85	50.86	1.794	043	9	22
13.72		6.449	001	1	0	50.87		1.793	204	21	
15.11	15.12	5.857	111	6	7	51.46	51.46	1.774	341	6	5
19.35	19.36	4.583	021	2	2	51.59	51.58	1.770	442	2	5
21.05	21.06	4.217	201	57	62	52.40	52.40	1.745	242	4	3
22.56	22.56	3.939	111	17	18	53.31	53.30	1.717	133	1	1
23.09	23.10	3.849	200	5	7	54.00	54.00	1.697	512	2	2
23.50	23.50	3.783	130	76	79	54.77	54.78	1.675	353	5	4
24.56	24.58	3.621	131	15	15	55.58	55.58	1.652	172	3	2
25.13	25.14	3.540	221	11	12	56.38		1.631	351	7	
25.74	25.74	3.458	112	49	49	56.45	56.40	1.629	080	2	5
26.88	26.88	3.314	220	100	100	56.51		1.627	334	1	
27.18	27.18	3.278	202	59	66	57.97	57.98	1.590	324	5	4
27.35	27.35	3.258	040	28	41	58.96	58.96	1.565	024	6	4
27.64	27.64	3.225	002	77	77	59.37	59.36	1.555	223	1	2
29.82	29.82	2.994	131	57	53	60.40	60.40	1.531	533	7	5
30.50	30.52	2.928	222	7	9	60.55	60.56	1.528	063	2	4
30.72	30.72	2.908	041	24	23	61.10	61.10	1.515	461	7	5
30.92	30.90	2.890	022	11	14	61.80	61.80	1.500	280	19	12
32.10		2.786	311	1	0	62.94	62.94	1.475	514	3	2
32.34	32.34	2.766	132	23	21	63.67	63.68	1.460	173	3	2
34.47	34.48	2.599	312	16	15	64.12	64.12	1.451	530	3	3
34.76	34.78	2.578	221	4	34	64.36	64.36	1.446	114	3	3
34.77		2.578	241	35		64.66	64.82	1.440	460	2	6
35.22	35.22	2.546	112	8	8	64.81		1.437	243	7	
35.63	35.64	2.518	310	8	7	65.00	64.98	1.434	463	2	5
36.09	36.10	2.487	240	3	3	65.16	65.16	1.430	552	2	3
37.09	37.10	2.422	151	8	7	65.39	65.40	1.426	602	6	5
37.70	37.70	2.384	331	12	10	65.55	65.56	1.423	190	2	4
38.82	38.82	2.318	113	7	6	66.55	66.56	1.404	402	6	3
39.78	39.78	2.264	332	4	3	67.33	67.34	1.389	405	2	2
40.44	40.46	2.228	132	1	2	67.53	67.54	1.386	553	2	3
40.46		2.228	223	1		67.70	67.70	1.383	264	3	3
40.81	40.90	2.209	330	2	4	69.06	69.06	1.359	325	2	1
40.91		2.204	151	3		69.61	69.62	1.349	621	2	2
41.55	41.56	2.172	060	25	20	70.02	70.02	1.343	192	5	3
41.99		2.150	003	1	0	71.01	71.02	1.326	604	2	1
42.47	42.48	2.127	241	11	9	72.03	72.04	1.310	135	4	3
42.70	42.70	2.116	401	4	6	72.28	72.30	1.306	245	2	4
42.85	42.84	2.109	402	5	7	72.35		1.305	531	2	
43.68		2.070	133	1	0	72.79	72.78	1.298	204	2	3
43.78	43.84	2.066	202	2	5	73.39	73.40	1.289	482	8	6
43.83		2.064	311	3		73.79	73.78	1.283	600	2	2
43.96	43.94	2.058	061	5	6	74.06	74.06	1.279	282	8	6
45.16	45.16	2.006	422	13	10	74.12		1.278	445	2	
46.05	46.06	1.969	222	11	8	74.62	74.64	1.271	392	2	3
46.47	46.48	1.952	333	3	3	74.66	74.64	1.270	641	2	3
47.19	47.20	1.924	400	10	10	75.70	75.72	1.255	535	2	3
47.20		1.924	351	3		75.75		1.255	355	2	
47.60	47.60	1.909	403	6	5	79.01	79.00	1.211	2102	2	2
48.06	48.06	1.891	260	2	2	80.63	80.60	1.191	316	2	2
48.28	48.28	1.883	331	2	2	82.00	82.00	1.174	733	2	1
49.20	49.22	1.850	113	7	5	83.62	83.62	1.155	484	3	2
49.33	49.32	1.846	420	2	5	84.48	84.48	1.146	084	3	2
49.52		1.839	152	2	0	86.58	86.58	1.123	443	3	1
49.74	49.84	1.832	423	1	4	88.44	88.42	1.104	753	2	2
49.83		1.828	350	3		90.73	90.76	1.082	155	2	1
50.36	50.36	1.810	262	4	4	93.28	93.28	1.059	665	2	1

TABLE 8. CALCULATED POWDER DATA FOR CELSIAN--CuK α .

2 θ (h k l)	2 θ (PK)	d	h k l	I(INT)	I(PK)	2 θ (h k l)	2 θ (PK)	d	h k l	I(INT)	I(PK)
13.21	13.24	6.698	110	1	3	52.68	52.68	1.736	228	3	3
13.56	13.58	6.523	020	44	80	53.62	53.64	1.708	514	3	2
13.57		6.517	002	22		54.08	54.08	1.694	314	4	3
15.10	15.10	5.864	112	20	23	54.70	54.70	1.677	356	10	7
19.24	19.24	4.610	022	34	39	55.47	55.48	1.655	174	7	5
22.22	22.22	3.997	112	6	7	55.75	55.74	1.647	352	10	8
22.77	22.78	3.902	200	23	25	56.38	56.40	1.631	080	5	6
23.40	23.40	3.799	130	34	36	56.39		1.630	338	2	
24.53	24.54	3.625	132	24	26	57.89	57.90	1.591	428	7	6
25.04	25.04	3.553	222	42	44	57.93		1.591	334	2	
25.64	25.64	3.472	114	76	78	58.32	58.34	1.581	028	9	8
26.59	26.60	3.349	220	100	100	58.43	58.44	1.578	226	5	8
27.15	27.16	3.282	204	34	37	59.60	59.60	1.550	510	2	2
27.34	27.34	3.259	004	28	32	60.16	60.20	1.537	066	4	9
29.55	29.56	3.021	132	59	55	60.20		1.536	336	10	
30.63	30.64	2.917	042	29	29	60.62	60.74	1.526	374	3	8
30.64		2.915	024	3		60.73		1.524	462	9	
32.24	32.26	2.774	134	42	38	60.83	1.521	174	3		
34.26	34.40	2.615	222	6	24	61.59	61.58	1.505	280	16	10
34.39		2.606	314	22		62.83	62.84	1.478	518	5	3
34.68	34.70	2.584	242	43	57	63.24	63.24	1.469	530	4	4
34.71		2.582	114	23		63.44	63.44	1.465	118	2	6
35.14	35.14	2.551	310	12	12	63.44	1.465	176	4		
35.85	35.86	2.502	240	3	3	63.91	63.92	1.455	246	9	8
36.27	36.28	2.474	150	1	1	64.07	64.06	1.452	460	4	6
37.05	37.06	2.425	152	12	10	64.82	64.82	1.437	604	6	5
37.47	37.48	2.398	332	6	6	65.32	65.32	1.427	404	5	4
38.58	38.58	2.332	116	14	12	66.71	66.72	1.401	372	3	3
39.69	39.70	2.269	334	12	10	67.33	67.36	1.390	556	4	4
39.98	39.98	2.253	134	10	9	67.47	67.48	1.387	268	5	5
40.36	40.36	2.233	226	4	8	67.74	67.66	1.382	512	2	3
40.36		2.233	330	4		68.77	68.78	1.364	622	4	3
40.68	40.68	2.216	152	15	13	68.92	68.94	1.361	4210	4	4
41.50	41.50	2.174	060	21	18	69.89	69.90	1.345	194	7	4
41.82	41.82	2.158	316	5	6	71.16	71.16	1.324	532	4	3
42.03	42.02	2.148	242	9	9	71.41	71.40	1.320	1310	4	4
42.28	42.28	2.136	402	8	8	71.57	71.58	1.317	208	3	4
42.64	42.66	2.118	404	7	8	71.88	71.88	1.312	2410	4	3
42.76	42.76	2.113	154	8	11	72.38	72.52	1.305	0100	2	3
43.04	43.10	2.100	204	3	12	72.52		1.302	266	2	
43.10		2.097	312	12		73.18	73.18	1.292	484	8	6
43.45	43.46	2.081	136	6	6	73.47	73.44	1.288	284	6	6
43.86	43.88	2.062	062	8	9	73.83	73.84	1.282	642	4	4
43.89		2.061	026	4		73.98	74.00	1.280	4410	5	5
44.60	44.60	2.030	422	6	5	74.49	74.48	1.273	394	2	2
44.95	44.96	2.015	424	15	12	77.80	77.80	1.227	552	2	2
45.34	45.34	1.999	224	9	8	79.17	79.18	1.209	288	2	3
46.42	46.50	1.955	336	9	12	79.95	79.95	1.199	664	2	0
46.50		1.951	400	9		80.13	80.18	1.197	2610	2	5
46.93	46.94	1.934	262	6	6	80.22	80.22	1.196	3112	3	2
46.99		1.932	352	2		81.44	81.46	1.181	736	2	
47.51	47.60	1.912	406	3	8	83.50	83.50	1.157	408	4	2
47.59		1.909	332	9		83.87	83.86	1.153	088	4	3
48.51	48.52	1.875	116	7	5	85.00	85.02	1.140	1.112	2	4
48.86	48.86	1.862	354	6	6	85.02		1.140	446	4	
49.10	49.10	1.854	154	8	7	87.79	87.82	1.119	710	3	3
49.43	49.44	1.842	350	4	4	87.87		1.110	756	3	
50.30	50.41	1.813	264	4	0	89.51	89.52	1.094	1510	3	1
50.41		1.809	064	3		92.97	93.12	1.062	590	2	3
50.43	1.808	046	11	93.11	1.061	6610		3	3		
50.64	50.64	1.801	208	18	16	93.62	1.056	2108	2	0	
51.07	51.08	1.787	442	12	10	109.54	109.70	0.943	5514	2	1
52.09	52.10	1.754	156	2	2						

measured on a Norelco diffractometer. Two curves relating half-width to 2θ were established from measured traces of well-crystallized Si and $0.03\mu\text{m Al}_2\text{O}_3$.¹ A proportionality constant was found by measuring the half-width, on experimental feldspar patterns. For computation of I_{PK} in the tables, we have used a value of 0.13° at $40^\circ 2\theta$ on the assumption that it is a good approximation of the half-width in *average* patterns. Half-widths at other values of 2θ were obtained by interpolation or extrapolation from the two experimentally determined curves. The patterns displayed in Figures 1–6 are computed on the basis of the smaller half-width (0.11° at $40^\circ 2\theta$) and are slightly better resolved especially at high diffraction angles than those based on 0.13° .

An absolute scale factor (*ASF*) is listed for each feldspar in Table 1. It is a conversion factor by which the tabulated, relative I_{INT} can be placed on an absolute scale, e.g. for use in quantitative analysis. As used in this paper $ASF = I_1/V^2 I_{\text{REL}}$ where I_1 is the actual calculated value of the intensity which takes into account multiplicity, $|F|^2$, temperature factors, the Lorentz-polarization correction and the portion of the absorption correction that is angularly dependent; $I_{\text{REL}} = I_{\text{INT}}$, μ is the linear absorption coefficient; V is cell volume.

Peak height intensities are determined from the simulated traces. Where overlap of adjacent peaks occurs, the reported peak height intensity reflects the sum of all individual contributions at that $2\theta_{\text{PK}}$. Both K_{α_1} and K_{α_2} components of the intensity contribute to the simulated trace. With their increased separation with increasing 2θ , the K_{α_2} components overlap K_{α_1} of other hkl reflections and commonly produces higher peak maxima than would otherwise be expected. Because of the rapid increase of the half-widths and the density of peaks in the back-reflection region, individual peaks are rarely identifiable.

In preparing the accompanying tables,² both integrated and peak height intensities were normalized to a maximum of 100. Then only reflections whose integrated intensities met the following conditions were included: Tables 2–4, for $2\theta < 45^\circ$, $I_{\text{hkl}} \geq 1.0$, for $2\theta > 45^\circ$, $I_{\text{hkl}} \geq 1.5$ and for $2\theta > 60^\circ$, $I_{\text{hkl}} \geq 2.0$. Tables 5–8, for $2\theta < 45^\circ$, $I_{\text{hkl}} \geq 0.5$, for $2\theta > 45^\circ$, $I_{\text{hkl}} \geq 1.0$, and for $2\theta > 60^\circ$, $I_{\text{hkl}} \geq 1.5$. Recorded $2\theta_{\text{PK}}$ and I_{PK} values, however, take all contributing reflections into account whether or not they meet the above criteria for inclusion in these tables. The $2\theta_{\text{PK}}$ listed in

¹ The curves were based on data measured with 1° divergence and anti-scatter slits over the whole range, and a 0.003-in. receiving slit.

² To obtain a copy of the unabridged tables, order NAPS Document #00181 from ASIS National Auxiliary Publications Service, c/o CCM Information Sciences, Inc., 22 West 34th Street, New York, New York 10001; remitting \$1.00 for microfiche or \$3.00 for photocopy, payable to ASIS-NAPS.

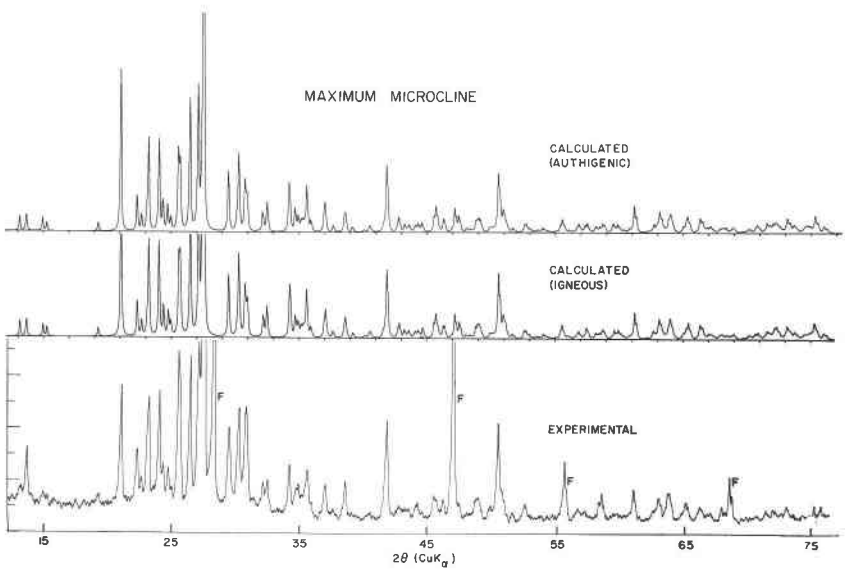


FIG. 1. Calculated and measured patterns for maximum microcline, $\text{CuK}\alpha$. Blue Mtn., Ontario microcline, $a=8.578$, $b=12.961$, $c=7.221$, $\alpha=90^\circ 39.9'$, $\beta=115^\circ 58.7'$, $\gamma=87^\circ 38.2'$. Measured pattern and cell parameters by D. B. Stewart. F=fluorite.

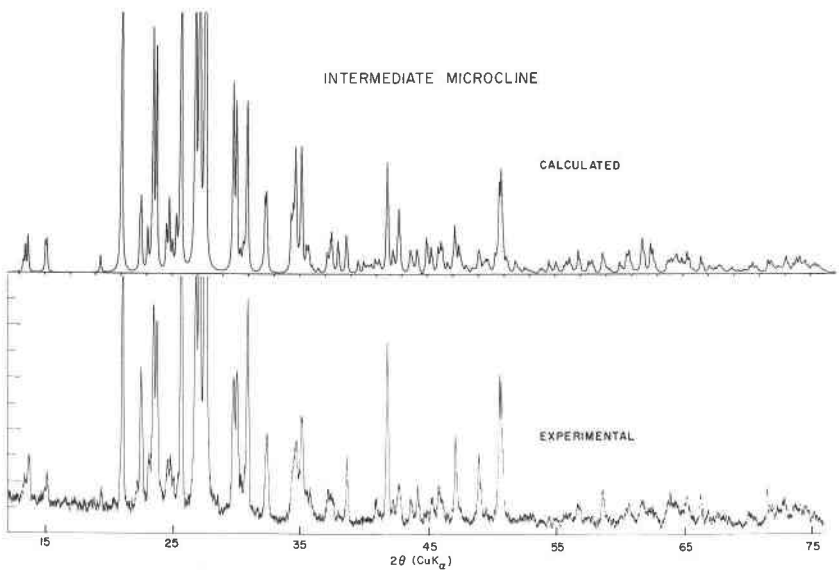


FIG. 2. Calculated and measured patterns for intermediate microcline, $\text{CuK}\alpha$. Spencer U, $a=8.578$, $b=12.957$, $c=7.213$, $\alpha=90^\circ 15.1'$, $\beta=116^\circ 1.6'$, $\gamma=89^\circ 13.5'$ -(Wright and Stewart, 1968). Measured patterns by D. B. Stewart.

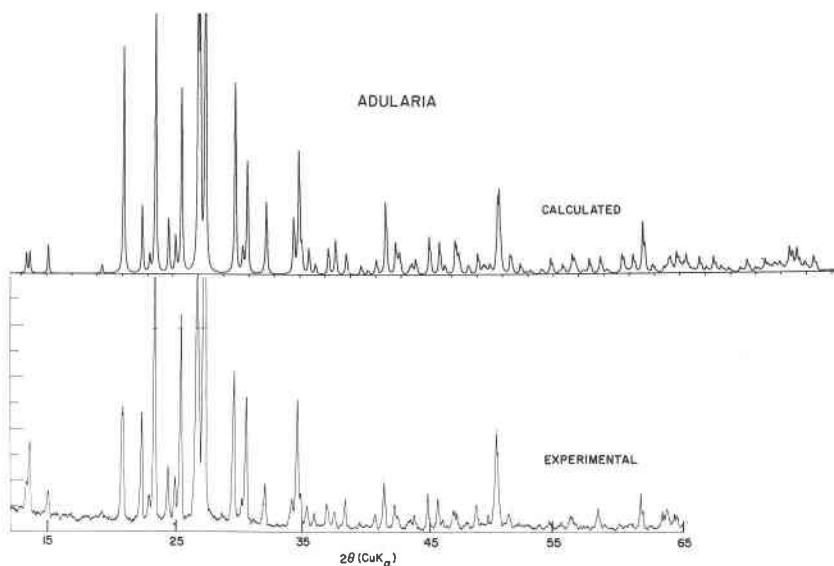


FIG. 3. Calculated and measured patterns for adularia, $\text{CuK}\alpha$. Spencer B; parameters given in Table 1. Measured pattern by D. B. Stewart.

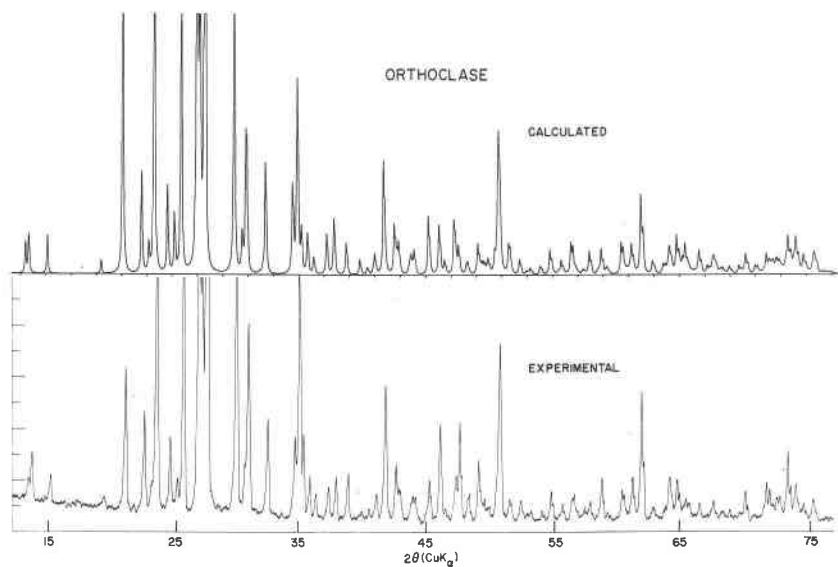


FIG. 4. Calculated and measured patterns for orthoclase, $\text{CuK}\alpha$. Spencer C equivalent from Bearpaw Mts., Mont. $a=8.561$, $b=12.995$, $c=7.194$, $\beta=115^\circ 59.6'$ (Wright and Stewart, 1968). Measured pattern by D. B. Stewart.

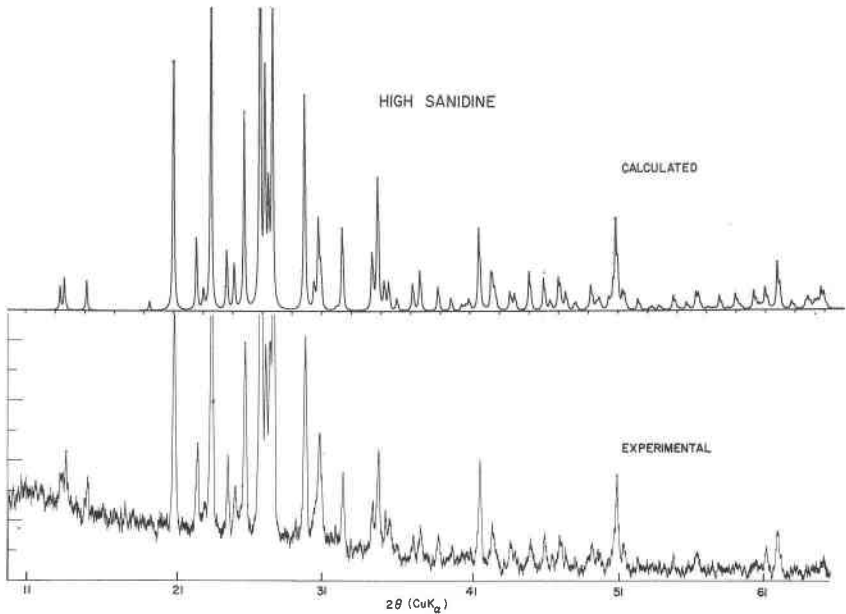


FIG. 5. Calculated and measured patterns for high sanidine, $\text{CuK}\alpha$. Or 100 synthesized from glass, 800°C , 2 kbars, 1 week. $a=8.603$, $b=13.021$, $c=7.178$, $\beta=116^\circ 0.6'$. Measurements and cell parameters by D. B. Stewart.

the tables is the position of the intensity maximum in the simulated trace *nearest* to the ideal $2\theta_{hkl}$. The I_{PK} listed is found by the computer from the digital representation of the simulated trace. By starting at the ideal $2\theta_{hkl}$ the computer searches for the nearest intensity maximum (I_{PK}) by moving in the direction of increasing intensity. The $2\theta_{PK}$ is the position corresponding to that I_{PK} . Under some conditions the position of I_{PK} may be more than one half-width from the initial $2\theta_{hkl}$. When this occurs,

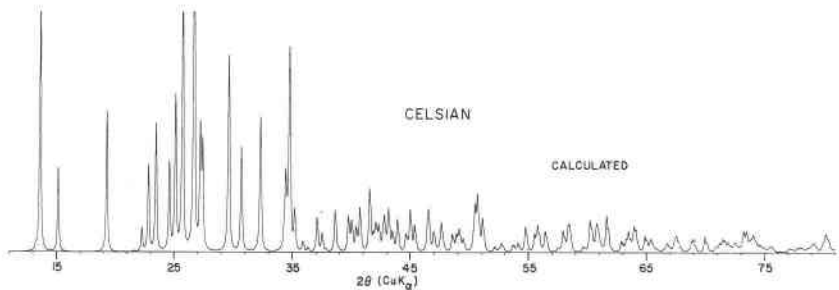


FIG. 6. Calculated pattern for celsian, $\text{CuK}\alpha$. Parameters as in Table 1.

the hkl is considered to be unresolved, and the corresponding I_{PK} is set to 0, e.g. 040 in Table 6. To emphasize that the hkl does in fact influence I_{PK} of the nearest peak to some degree, the appropriate $2\theta_{hkl}$'s are bracketed, e.g. 27.43° and $27.58^\circ 2\theta$ in Table 6.

In most instances the listed hkl 's, i.e. those that pass the I_{INT} test for inclusion, make the largest contribution to the intensity of the associated peak. However in some instances (e.g. 2.12.3 at $118.42^\circ 2\theta$, Table 5, $\bar{2}64$ at $67.26^\circ 2\theta$, Table 3, and 600 at $73.84^\circ 2\theta$ in Table 6) its contribution may be negligible with respect to the total contribution of several overlapping weaker reflections. $2\theta_{PK}$'s are located to the nearest $0.02^\circ 2\theta$. All $2\theta_{hkl}$ values are based on $\lambda = 1.54050$ ($\text{CuK}\alpha_1$).

Table 9 contains a summary of the indices associated with the five strongest I_{INT} and I_{PK} computed for each pattern. The values of the intensities are given in parentheses. The problem of overlap in complex patterns is evident in the data of Table 9. Not only do weak reflections superimpose to produce strong peaks, but as cell dimensions change, the degree of overlap also changes and the patterns show distinct shifts in relative intensities for similar peaks.

TABLE 9. INDICES AND INTENSITIES OF FIVE STRONGEST CALCULATED REFLECTIONS (I_{INT}) AND PEAKS (I_{PK}), $\text{CuK}\alpha_1$

	I_{INT}					I_{PK}				
	1	2	3	4	5	1	2	3	4	5
Igneous Maximum Microcline	002 (100)	$\bar{2}01$ (76)	$\bar{2}02$ (73)	220 (67)	$\bar{2}20$ (62)	$\left\{ \begin{matrix} \bar{2}20 \\ 002 \\ 040 \\ 100 \end{matrix} \right\}$	$\bar{2}01$ (51)	$\bar{2}02$ (48)	220 (41)	130 (30)
Authigenic Maximum Microcline	002 (100)	$\bar{2}01$ (74)	$\bar{2}02$ (72)	220 (67)	$\bar{2}20$ (62)	$\left\{ \begin{matrix} \bar{2}20 \\ 002 \\ 040 \\ 100 \end{matrix} \right\}$	$\bar{2}01$ (54)	$\bar{2}02$ (51)	220 (45)	130 (32)
Intermediate Microcline	002 (100)	201 (74)	$\bar{2}02$ (73)	$\bar{2}20$ (70)	220 (67)	$\left\{ \begin{matrix} \bar{2}20 \\ \bar{2}02 \\ 040 \end{matrix} \right\}$	$\left\{ \begin{matrix} 002 \\ 040 \end{matrix} \right\}$	201 (58)	$\bar{2}20$ (53)	$\left\{ \begin{matrix} \bar{1}\bar{1}2 \\ \bar{1}12 \end{matrix} \right\}$ (47)
Adularia	220 (100)	002 (78)	130 (72)	$\bar{2}01$ (59)	131 (57)	220 (100)	$\left\{ \begin{matrix} 002 \\ 002 \end{matrix} \right\}$ (100)	$\bar{2}02$ (75)	130 (72)	$\bar{2}01$ (61)
Orthoclase	220 (100)	002 (78)	130 (74)	131 (59)	$\bar{2}02$ (59)	220 (100)	002 (82)	130 (75)	$\bar{2}02$ (67)	$\bar{2}01$ (61)
High Sanidine	220 (100)	002 (77)	130 (76)	$\bar{2}02$ (59)	$\bar{2}01$ (57)	220 (100)	130 (79)	002 (77)	$\bar{2}02$ (66)	$\bar{2}01$ (62)
Celsian	220 (100)	$\bar{1}14$ (76)	132 (59)	020 (44)	$\bar{2}42$ (43)	220 (100)	$\left\{ \begin{matrix} 020 \\ 002 \end{matrix} \right\}$ (80)	$\bar{1}14$ (78)	$\left\{ \begin{matrix} \bar{2}42 \\ 114 \end{matrix} \right\}$ (57)	132 (55)

DISCUSSION OF RESULTS

Calculated powder patterns are displayed in Figures 1–6 together with diffractometer traces of comparable or identical K-feldspars.¹ The agreement between the calculated and experimental patterns is best for synthetic high sandine (Fig. 5); this agreement is analogous to best matches between experimental patterns from synthetic plagioclases and their calculated counter-parts (Borg and Smith, 1968). The purity of the materials and their fine grain size have minimized preferred orientations and eliminated the chief sources of discrepancy. Nonetheless, there is good agreement between all juxtaposed patterns. Preferred orientation related to cleavage would be expected to enhance intensities of $00l$, $0k0$ and $0kl$ peaks and to diminish those of $h00$, and to lesser extent $h0l$ and $hk0$ in the experimental patterns relative to the calculated; however the effect of preferred orientation on intensity of general hkl planes is less predictable. Differences in peak heights tend to follow the general pattern, e.g., 201 and $\bar{2}01$ are consistently low in all experimental traces, and the 001 – 020 peak is consistently high. In Figure 4, the difference in relative peak heights at $2\theta \simeq 47.3^\circ$ is again related to preferred orientation. In the experimental pattern, 403 is stronger than 400 whereas the converse is true in the calculated pattern. Other differences such as 111 and/or $\bar{1}\bar{1}\bar{1}$ peaks in Figures 2 and 3 ($2\theta \simeq 22.5^\circ$) are not easily explained.

Peak resolution is superior in the calculated patterns and can be improved by plotting on expanded scales. This is comparable in diffractometry to scanning at a slower speed and higher time constants. The calculated traces do not take into account the common diffractometry practice of changing to larger divergence and antiscatter slits at higher 2θ values. For greater resolution in the back reflection regions, the Debye-Scherrer technique may be more useful because of 1) the different relationship between half-width and 2θ and 2) the intensity enhancement due to the lower absorption effect in the back reflections than in the front reflections.

The calculated K-feldspar patterns readily illustrate criteria whereby the various polymorphs can be distinguished and aid indexing of observed peaks prior to data reduction leading to precise cell and obliquity parameters. There is continuous variation between adjacent K-feldspars of Table 1, and the distinction, for example, between a low sandine and orthoclase can be difficult. Nonetheless, clear qualitative differences in powder patterns of the end members permit them to be recognized at a

¹ All experimental patterns are by D. B. Stewart who used glass slide mounts, $\text{CuK}\alpha$ radiation, pulse-height discrimination, and the following instrumental settings: 45 kV, 20 mA, $2^\circ/\text{min}$ TC = 4 sec, 0.006-in. receiving slits, and 1° divergent and anti-scatter slits.

glance. Patterns of the triclinic K-feldspars are distinguished from the monoclinic by splitting of related reflections such as $130\bar{1}30$ and 131 and $1\bar{3}1$. The splitting increases with obliquity as a result of Al/Si order. The pattern of monoclinic high sanidine differs from those of adularia and orthoclase by the presence of four rather than three distinct peaks corresponding to 220, $20\bar{2}$, 040 and 002 near $2\theta \sim 27^\circ$. The 002 and 040 reflections in orthoclase are, in fact, separated by 0.15° (Table 10) but they are not clearly resolved in either the experimental or calculated patterns. Because of the effect of Al/Si ordering on cell parameters, the spacing between these two lines is a measure of the degree of Al/Si order in the monoclinic varieties; all other variables such as Na-content being equal. The proposal to use c^*/b^* ratios to assess Al/Si order in both mono-

TABLE 10. SEPARATION OF 002 AND 040 IN MONOCLINIC K-FELDSPARS

<i>hkl</i>	High Sanidine	Orthoclase	Adularia
	2θ (peak)	2θ (peak)	2θ (peak)
220	26.88	26.91	26.94
$20\bar{2}$	27.18	27.14	27.10
040	27.35	27.58	27.52
002	27.64		
$\Delta 2\theta$ 040 - 002	0.29°	0.15°	0.04°
for $\text{CuK}_{\alpha 1}$	4 peaks	3 peaks	3 peaks

clinic and triclinic varieties (Jones, 1966) must by necessity, be based on calculated 002 and 040 spacings since they are commonly unresolved in all triclinic and some monoclinic varieties.

Many other parameters, based on unit-cell size and shape have been suggested to estimate Al/Si disorder. Separations of 130 and $1\bar{3}0$ or 131 and $1\bar{3}1$ in triclinic varieties have proven useful in part due to the fact that these reflections are strong, and there is little or no interference from adjacent reflections at any composition. In maximum microcline, 200 overlaps 130 (Orville, 1967, p. 83) but the relative intensities 7:44, together with the probable greater diminution of 200 than 130 with any degree of preferred orientation, minimizes the problem. Other pairs of *hkl* reflections, e.g., 280 and $2\bar{8}0$ or 222 and $2\bar{2}2$, might be proposed as suitable criteria for the determination of Si/Al order on the basis of the data in Tables 2-7. By virtue of their larger separation, they are more sensitive to changes in obliquity although they are generally moderate to weak reflections.

Wright's (1968) "three-peak" method for determining composition and structural state in K-feldspars is based on the positions of 201 , 060

and $\bar{2}04$. From Tables 2-7, it can be seen that $\bar{2}01$ and 060 are, for all practical purposes, not overlapped by other hkl 's. On the other hand, $\bar{2}04$ may be overlapped and its 2θ position affected by as many as four unresolvable and weak $k\bar{l}0$ and hkl reflections (maximum microcline), the total of whose intensity in a randomly oriented mount approaches that of $\bar{2}04$ (orthoclase). Clearly, it is desirable to eliminate preferred orientation in a sample before measuring the precise positions of these peaks. Otherwise the likely diminution of the $h0l$'s, particularly of $\bar{2}04$, and enhancement of $0kl$'s may introduce unnecessary difficulties in both their recognition and measurement.¹

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Note added in proof—The crystallographic setting used by Bailey and Taylor (1955) is in the old setting for intermediate microcline, and the resulting Miller indices are inconsistent with modern usage. The proper setting $\alpha(\text{new}) = 180^\circ - \alpha(\text{old})$, $\gamma(\text{new}) = 180^\circ - \gamma(\text{old})$, results in an indexing change from hkl to $\bar{h}\bar{k}\bar{l}$, and all indices in Table 4 should be changed accordingly.

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¹ In practice, such difficulties are rarely encountered (D. B. Stewart, personal communication); however, they remain potential problems in the maximum microcline.

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