

about the validity of such simple considerations as those used here, he is nevertheless gratified to find how well they do explain phenomena that must really be based on very complex systems of chemical forces.

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REFERENCES

- BOWEN, N. L. AND TUTTLE, O. F. (1950), The system $\text{NaAlSi}_3\text{O}_8$ — $\text{K AlSi}_3\text{O}_8$ — H_2O : *Jour. Geol.*, **58**, 489–511.
- COLE, W. F., SORÜM, H. AND KENNARD, O. (1949), The crystal structures of orthoclase and sanidinized orthoclase: *Acta Cryst.*, **2**, 280–287.
- COOMBS, D. S. (1954), Ferriferous orthoclase from Madagascar: *Mineral. Mag.*, **30**, 409–427.
- FERGUSON, R. B., TRAILL, R. J., AND TAYLOR, W. H. (1958), The crystal structures of low-temperature and high-temperature albite: *Acta Cryst.*, **11**, 331–348.
- HOWIE, R. A. (1955), The geochemistry of the charnockite series of Madras, India: *Trans. Roy. Soc. Edinburgh*, **62**, 725–768.
- LAVES, F. (1952), Phase relations of the alkali feldspars: *Jour. Geol.*, **60**, 436–450, 549–574.
- LAVES, F. AND SOLDATOS, K. (1961), Die Albit/Mikroklin-Orientierungs-Beziehungen und ihre genetische Deutung: *Zeit. Krist.*, in press.
- MACKENZIE, W. S. AND SMITH, J. V. (1955), The alkali feldspars I: *Am. Mineral.*, **40**, 707–732.
- AND ——— (1956), The alkali feldspars III: *Am. Mineral.*, **41**, 405–427.

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INDEXED POWDER DIFFRACTION DATA FOR SCAPOLITE

GERALD V. GIBBS, *Metallurgy Research Laboratory, Norris, Tenn.*

AND

F. DONALD BLOSS, *Dept. of Geology, Southern Illinois University, Carbondale, Ill.*

During a study of the similarities between natural scapolites and fibrous potassium lead silicates synthesized by Shell (1957), no indexed powder diffraction data for scapolite for comparison could be found in the literature nor in the x -ray powder data file. Recently, Eugster and Prostka (1960, p. 1859) published data on seven indexed peaks for two synthetic scapolites. However, it is felt that additional indexed data, particularly for natural scapolites, might be a desirable addition to the literature since future comparisons might be desired. This note thus presents indexed data for some 40 peaks for scapolites from Arendal, Norway and from Grenville, Quebec.

TABLE 1. X-RAY POWDER DIFFRACTION DATA FOR SCAPOLITE

Arendal				Grenville			
<i>hkl</i>	<i>d</i> _{obs}	<i>I</i> / <i>I</i> ₀	<i>d</i> _{calc}	<i>hkl</i>	<i>d</i> _{obs}	<i>I</i> / <i>I</i> ₀	<i>d</i> _{calc}
110	8.556	5	8.553	110	8.600	5	8.605
101	6.439	5	6.419	200	6.087	20	6.085
200	6.040	20	6.048	211	4.422	<5	4.419
211	4.397	5	4.402	220	4.306	5	4.303
220	4.282	10	4.276	310	3.846	45	3.849
310	3.824	60	3.826	301	3.577	10	3.577
301	3.558	20	3.560	112	3.465	95	3.465
112	3.464	100	3.463	202	3.210	10	3.214
321	3.069	70	3.067	321	3.085	75	3.083
400	3.027	55	3.024	400	3.043	55	3.043
222	2.833	10	2.835	330	2.869	<5	2.869
411	2.734	15	2.736	222	2.843	<5	2.842
420	2.703	25	2.705	411	2.750	5	2.750
312	2.693	30	2.691	420	2.721	5	2.722
510	2.370	<5	2.372	312	2.700	100	2.699
431	2.306	15	2.304	510	2.387	<5	2.387
332	2.278	5	2.277	431	2.317	15	2.317
422	2.204	5	2.201	332	2.287	15	2.286
521	2.152	10	2.153	422	2.209	<5	2.209
303	2.141	20	2.140	521	1.164	15	2.165
530	2.074	5	2.073	303	2.142	20	2.143
611	1.932	15	1.923	530	2.086	5	2.087
620	1.912	30	1.912	512	2.091	10	2.019
004	1.892	10	1.893	611	1.933	15	1.935
541	1.832	5	1.833	620	1.923	30	1.925
532	1.820	5	1.819	413	1.918	15	1.918
631	1.753	10	1.754	004	1.893	15	1.893
710	1.712	15	1.711	541	1.843	10	1.844
640	1.677	5	1.677	532	1.827	<5	1.828
721	1.622	5	1.623	631	1.764	10	1.765
613	1.562	5	1.562	503}	1.752	<5	1.752
712	1.558	5	1.559	433}			
543	1.512	5	1.512	710	1.721	5	1.721
732	1.464	10	1.465	640	1.687	<5	1.688
325	1.381	<5	1.381	721	1.632	<5	1.633
624	1.346	15	1.345	404	1.607	<5	1.607
910	1.335	<5	1.336	613	1.567	15	1.568
653	1.319	<5	1.320	543	1.518	<5	1.518
921}	1.293	<5	1.293	811}	1.514	5	1.514
761}				741}			
435}	1.284	<5	1.284	732	1.472	10	1.472
505}				505	1.459	5	1.459
				325	1.381	<5	1.381
				822	1.376	15	1.375
				624	1.349	5	1.349
				910	1.344	<5	1.344
				653	1.325	<5	1.326
				921}	1.301	<5	1.301
				761}			
				505}	1.286	5	1.286
				435}			

The Arendal scapolite was white in color and non-fluorescent whereas the Grenville scapolite was yellow and fluoresced a brilliant canary yellow under long wave ultraviolet radiation. Each scapolite was mottled with

less transparent areas which, when examined as grains under the polarizing microscope, appeared to contain a finely dispersed alteration product. Thus it was necessary to coarse-crush each scapolite and isolate the clear grains, then crush these clear grains to -400 mesh for the x -ray and chemical analysis. Smear mounts of the -400 mesh crushed fragments of each scapolite were scanned at $\frac{1}{4}$ degree per minute with a Norelco high-angle diffractometer operated in conjunction with an automatic strip chart recorder. Instrumental settings were: divergence and scatter slits, 1 degree; receiving slits, 0.006 inches; strip chart scale, $\frac{1}{2}$ degree per inch; time constant, 4; multiplier, 1; scale factor, 8 and 16; filtered $\text{CuK}\alpha$ radiation.

The 2θ values for resolved $\text{K}\alpha_1$ peaks on the strip charts were read at the midpoints at $\frac{2}{3}$ the height of the peak (Donnay and Donnay, 1951); the 2θ values for unresolved or partly resolved peaks were read at the midpoints at $\frac{1}{2}$ the height of the peak (Smith and Sahama, 1954). These

TABLE 2. CHEMICAL ANALYSIS AND CALCULATION OF THE UNIT CELL
CONTENT OF THE ARENDAL SCAPOLITE
(Analyst R. E. Hooper) U. S. Bureau of Mines, Norris, Tenn.

	Analysis wt. %	Mass units per unit cell (atomic-wt. units)	Gram-molecular wt. of oxide, or constituent of column 1	No. of oxides, etc. per unit cell	No. of metal ions per unit cell	No. of anions per unit cell
SiO_2	50.38	894.48	60.06	14.89	14.89	29.78
Al_2O_3	24.18	429.31	101.94	4.21	8.42	12.63
Fe_2O_3	0.29	5.15	159.70	0.03	0.06	0.09
TiO_2	0	—	—	—	—	—
CaO	13.06	231.88	56.08	4.13	4.13	4.13
MgO	0	—	—	—	—	—
Na_2O	7.09	125.88	61.97	2.03	4.06	2.03
K_2O	0.51	9.06	94.20	0.10	0.20	0.10
CO_2	0.94	16.69	44.01	0.38	0.38	0.76
Cl	4.32	76.70	35.46	2.16	—	2.16
F^-	0.31	5.50	19.00	0.29	—	0.29
SO_3	0	—	—	—	—	—
H_2O	n.d.	—	—	—	—	—
	101.07					
Less O	.13					
equivalent to F and Cl, resp.	.95					
	99.99 ¹					

¹ The total reported by the analyst, *i.e.* 100.25%, has been readjusted to 100.00%.

peak readings were then corrected to an internal standard—a synthetic spinel (MgAl_2O_4) with cell dimensions that had been carefully determined with respect to transistor grade silicon.

The data of Table 1 for the Arendal specimen were indexed on the basis of a tetragonal, body-centered cell: a 12.095, c 7.571A \pm 0.05%; for the Grenville on a similar cell: a 12.163, c 7.569A \pm 0.05%. In the case of the former precession photographs were taken to confirm the diffraction indices assigned to the peaks of the powder diffraction record. These photographs exhibited the symmetry $4/m$ and a systematic absence of reflections with $h+k+l$ odd. The space groups consistent with these diffraction data are $I4$, $I\bar{4}$ and $I4/m$. Piezoelectric tests were made on the Arendal scapolite as a possible means of discerning whether scapolite possesses space group symmetry $I4$, $I\bar{4}$ (noncentric), or $I4/m$.

TABLE 3. CHEMICAL ANALYSIS AND CALCULATION OF THE UNIT CELL CONTENT OF THE GRENVILLE SCAPOLITE
(Analyst R. E. Hooper)

	Analysis wt. %	Mass units per unit cell (atomic wt. units)	Gram-molecular wt of oxide, or constituent of column 1	No. of oxides, etc. per unit cell	No. of metal ions per unit cell	No. of anions per unit cell
SiO_2	44.46	806.74	60.06	13.43	13.43	26.85
Al_2O_3	29.14	528.75	101.94	5.19	10.38	15.57
Fe_2O_3	0.23	4.17	159.70	0.03	0.06	0.09
TiO_2	0	—	—	—	—	—
CaO	16.36	296.87	56.08	5.29	5.29	5.29
MgO	0	—	—	—	—	—
Na_2O	2.43	44.09	61.97	0.71	1.42	0.71
K_2O	2.23	40.46	94.20	0.43	0.86	0.43
CO_2	0.95	17.24	44.01	0.39	0.39	0.78
Cl	0.35	6.35	35.46	0.18	—	0.18
F^-	0.15	2.72	19.00	0.14	—	0.14
SO_3	1.07	19.42	80.07	0.24	0.24	0.72
H_2O^-	0.11	—	—	—	—	—
H_2O^+	2.66	48.27	18.02	2.68	5.36	2.68
	100.14					
Less O equivalent to F and Cl	.06 .08					
	100.00 ¹					

¹ The total reported by the analyst, *i.e.* 100.16%, has been readjusted to 100.00%.

(centric).* The test was made at 50° intervals between 20° C. and the boiling temperature of liquid nitrogen with the piezoelectric detector at the Pennsylvania State Crystallographic Laboratory, University Park, Pennsylvania. The results of the tests gave no indication of non-centrosymmetry, although it is realized that a negative result is not conclusive. However, Professor Pepinsky is of the opinion that the piezoelectric detector used for the test is very sensitive and that a negative result is a good indication of centrosymmetry. Thus, it appears probable that scapolite belongs to the centrosymmetric space group $I4/m$ which is in agreement with Pauling's (1930) postulated structure for scapolite. However, definite confirmation of this conclusion will have to await a detailed structural analysis of scapolite.

Other physical constants measured for these scapolites were, for the Arendal scapolite: ω_D 1.566, ϵ_D 1.544, ρ 2.66 and for the Grenville scapolite: ω_D 1.588, ϵ_D 1.559, and ρ 2.69.

The unit cell content of the two scapolites was found by calculating the atomic-weight units in the unit cell from the relation $\rho V/1.66$ and allocating these units to the various oxides, etc., on the basis of their respective weight percentages reported in the chemical analysis (Tables 2 and 3). The notation ρ and V refer to the measured density and unit cell volume, respectively, of the scapolites. No determination of H₂O was made in the chemical analysis of the Arendal scapolite because the 1.89 gm sample available for the analysis was expended in the analytical determination of the other chemical constituents.

REFERENCES

- BURLEY, B. J., FREEMAN, E. B. AND SHAW, D. M. (1961), Studies on Scapolite: *Canadian Mineral.* **6**, 670-679.
- DONNAY, G. AND DONNAY, J. D. H. (1952), The Symmetry Change in the High-Temperature Alkali-Feldspar Series: *Am. J. Sci.*, **Bowen Vol.**, 118.
- EUGSTER, H. P. AND PROSTKA, H. J. (1960), Synthetic Scapolites: *Proc. G.S.A., Denver*, Abstract, p. 92.
- GIBBS, G. V. AND LEWIS, R. M. (in press), Quadratic Functions for Copper Radiation -0° to $180^\circ 2\theta$.
- PAULING, L. (1930), The Structure of Some Sodium and Calcium Alumino-Silicates: *Proc. Nat. Acad. Sci.*, **16**, 453.
- SHELL, H. R. (1957), Synthetic Asbestos Investigations III. Synthesis and Properties of Fibrous Potassium-Lead Silicate: *Department of the Interior, Bureau of Mines Report of Investigations* 5293.
- SMITH, J. V. AND SAHAMA, TH. C. (1954), Determination of the Composition of Natural Nephelines by an X-Ray Method: *Min. Mag.*, **XXX**, No. 226, 440.

* While this article was in press, "Studies on Scapolite" by B. J. Burley, E. B. Freeman and D. M. Shaw appeared in *Canad. Mineral.* **6**, part 5, 670-679, with powder photograph data and a discussion of symmetry.