

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.

Thanks are expressed to Drs. J. R. Goldsmith, F. Laves and W. S. MacKenzie for critical examination of the manuscript and to the National Science Foundation for support from grant G14467.

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THE AMERICAN MINERALOGIST, VOL. 46, NOVEMBER–DECEMBER, 1961

INDEXED POWDER DIFFRACTION DATA FOR SCAPOLITE

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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> | d_{obs} | I/I_0 | d_{calc} | <i>hkl</i> | d_{obs} | I/I_0 | d_{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} | | | | 811} | | | |
| 761} | 1.293 | <5 | 1.293 | 741} | 1.514 | 5 | 1.514 |
| 435} | | | | 732 | 1.472 | 10 | 1.472 |
| 505} | 1.284 | <5 | 1.284 | 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} | | | |
| | | | | 761} | 1.301 | <5 | 1.301 |
| | | | | 505} | | | |
| | | | | 435} | 1.286 | 5 | 1.286 |

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 H_2O 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.

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* 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.