OBSERVATIONS ON SOME ALUMINIUM FLUORIDE MINERALS[1]

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ABSTRACT

Jarlite ($G=3.87$) is monoclinic, tabular on (001); space-group $C2/m$, $C2$, or Cm; $a=15.99$, $b=10.82$, $c=7.24$ kX, $\beta=101°\ 49'$; $Y=b$, $Z{:}c=+(84°\pm2°)$; $\alpha=1.430$, $\beta=1.435$, $\gamma=1.437$, $2V=90°\pm10°$; the composition $NaSr_3Al_3F_{16}$ is apparently in error. "Metajarlite" ($G=3.65$, with inclusions), with $\alpha=1.429$, $\beta=1.431$, $\gamma=1.434$, and an *x*-ray powder pattern very like that of jarlite, is merely a variety of jarlite. Prosopite is monoclinic, $C2/c$; $a=6.67$, $b=11.17$, $c=7.37$ kX, $\beta=94°\ 56'$. Weberite is orthorhombic, *Ibmm* or *Ibm*2; the unit cell with $a=7.30$, $b=7.05$, $c=9.97$ kX, contains $4[Na_2MgAlF_7]$; $X=a$, $Y=b$. Cryolithionite has $a=12.14$ kX. Powder photographs of ralstonite show indications of non-cubic symmetry, and "hagemannite" is an ochre consisting of ralstonite with some thomsenolite and goethite. *X*-ray powder spacings and intensities (10 scale) are given for gearksutite and ralstonite, and similar data with indices and calculated spacings are given for cryolite, jarlite and "metajarlite," prosopite, and weberite. All the material studied, except prosopite from Colorado, came from Ivigtut, Greenland.

Occurring with the cryolite at the most famous locality, Ivigtut, Greenland, are representatives of most of the rare aluminium fluoride minerals. An excellent suite of specimens from the Ivigtut quarry was kindly made available to the author by Professor H. S. Scott of the Department of Geology, McMaster University, Hamilton, Ontario. Professor Scott had collected these specimens at Ivigtut in 1942 when, as geologist for Mr. Hans Lundberg of Toronto, he made a geological examination of the cryolite deposit. A crystallographic investigation of the lesser known aluminium fluoride minerals in this suite was carried out in the Mineralogical Laboratory of the Department of Geological Sciences, University of Toronto, under the helpful and stimulating direction of Professor M. A. Peacock. Some of the results of this investigation, those on thomsenolite and pachnolite, have already been published (Ferguson, 1946); the present paper summarizes the new and confirmatory observations on the remaining minerals. The essence of this paper was presented before the Mineralogical Society of America at the 1947 meeting in Ottawa and has been published in abstract (Ferguson, 1948).

Detailed studies were made of jarlite $NaSr_3Al_3F_{16}$(?) and weberite Na_2MgAlF_7 as well as thomsenolite and pachnolite, both $NaCaAlF_6\cdot H_2O$; a small amount of work, mainly indexing the *x*-ray powder photographs, was carried out on the remaining minerals in the group (excluding

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elpasolite K_2NaAlF_6 which has not been reported from Ivigtut): cryolite Na_3AlF_6, chiolite $Na_5Al_3F_{14}$, cryolithionite $Na_3Li_3Al_2F_{12}$, gearksutite $CaAl(F,OH)_5 \cdot H_2O$, prosopite $CaAl_2(F,OH)_8$ (from Colorado), ralstonite $Na_{2-x}(Al,Mg)_2(F,OH)_6 \cdot 1-yH_2O$.

All *x*-ray diffraction photographs were taken with Cu radiation, a Ni filter being used for the powder pictures. Results are given in kX units ($CuK\alpha_1 = 1.5374$ kX). Intensities were visually estimated on a scale of 10.

CRYOLITE—Na_3AlF_6

An *x*-ray powder photograph of this mineral indexed well on the cell dimensions of Menzer (1928). The powder data indexed to $\theta(Cu) = 29.35°$ appear in Table 1, and agree well with the only previously published data (unindexed) in the ASTM Card Index (1943, card 3469).

CRYOLITHIONITE—$Na_3Li_3Al_2F_{12}$

Menzer (1930) has published powder data for this cubic mineral indexed on a cell edge of 12.097 Å. A new powder photograph gave slightly

TABLE 1. CRYOLITE—Na_3AlF_6: *X*-RAY POWDER PATTERN
Monoclinic, $P2_1/n$; $a=5.39$, $b=5.59$, $c=7.76$ kX, $\beta=90°\ 11'$; Z=2

I	θ(Cu)	*d*(meas.)	(*hkl*)	*d*(calc.)	*I*	θ(Cu)	*d*(meas.)	(*hkl*)	*d*(calc.)
7	9.9°	4.47	(011) (101) $(\bar{1}01)$	4.536 4.427	4	21.65°	2.08	(122) $(\bar{1}22)$ (212) $(\bar{2}12)$	2.090 2.058
7	11.45	3.87	(110) (002)	3.880 3.880	10	23.35	1.939	(220) (004)	1.940 1.940
2	12.85	3.46	(111) $(\bar{1}11)$	3.470	1	24.0	1.890	(023) (221) $(\bar{2}21)$	1.898 1.882
9	16.25	2.75	(020) (112) $(\bar{1}12)$ (200)	2.795 2.744 2.695	½	25.5	1.786	(123) $(\bar{1}23)$	1.791
½	18.25	2.47	(120)	2.481	1	25.9	1.760	(130)	1.761
3	18.5	2.42	(210)	2.428	1	26.35	1.732	(114) $(\bar{1}14)$ (222) $(\bar{2}22)$	1.735 1.735
8	19.3	2.33	(013) (103) $(\bar{1}03)$ (211) $(\bar{2}11)$	2.348 2.332 2.317	4	26.7	1.711	(131) $(\bar{1}13)$ (310)	1.717 1.711
4	19.85	2.26	(022)	2.268	2	27.4	1.670	(311) $(\bar{3}11)$	1.670
1	20.35	2.21	(202) $(\bar{2}02)$	2.213	6	28.8	1.596	(024)	1.594
4	21.0	2.14	(113) $(\bar{1}13)$	2.152	8	29.35	1.568	(312) $(\bar{3}12)$	1.565

TABLE 1—*continued*

I	θ(Cu)	*d*(meas.)	*I*	θ(Cu)	*d*(meas.)	*I*	θ(Cu)	*d*(meas.)
½	30.75°	1.503	4	38.8°	1.227	2	48.8°	1.022
½	31.05	1.490	½	39.35	1.212	1	49.75	1.007
1	31.9	1.455	1	41.45	1.161	½	52.65	0.967
1	32.6	1.427	½	42.7	1.134	½	53.85	0.952
1	33.4	1.396	½	43.35	1.120	½	54.7	0.942
4	34.05	1.373	½	44.0	1.107	½	56.5	0.922
1	34.7	1.350	2	45.2	1.083	2	57.1	0.916
2	35.75	1.316	½	46.45	1.061	2	57.9	0.907
1	36.1	1.305	½	47.0	1.051	1	59.4	0.893
½	37.1	1.274	2	47.45	1.043	1	62.55	0.866
½	38.25	1.242	2	48.15	1.032			

larger spacings than Menzer's and led to a cell edge of 12.14 kX. Except for the small differences in spacing, the new indexed powder data agreed well with Menzer's.

GEARKSUTITE—$CaAl(F,OH)_5 \cdot H_2O$

This mineral occurs as white, earthy, kaolin-like masses at Ivigtut with thomsenolite and cryolite, and at several other localities in different association. Since macroscopic crystals are unknown, gearksutite does not permit of a single-crystal investigation which is necessary to interpret the complex powder pattern. Specimens of this mineral from Ivigtut and

TABLE 2. GEARKSUTITE—$CaAl(F, OH)_5 \cdot H_2O$: *X*-RAY POWDER PATTERN

I	θ(Cu)	*d*(meas.)	*I*	θ(Cu)	*d*(meas.)	*I*	θ(Cu)	*d*(meas.)
1	6.6°	6.69	1	21.4°	2.11	3	31.85°	1.457
2	8.45	5.23	4	21.75	2.07	2	32.4	1.435
10	9.75	4.54	½	22.5	2.01	1	33.5	1.393
1	11.75	3.77	½	23.0	1.967	4	34.3	1.364
3	12.6	3.52	8	23.55	1.924	½	35.9	1.311*b*
7	13.34	3.33*d*	3	23.85	1.901	2	37.35	1.267
8	14.15	3.14	3	25.0	1.819	3	38.45	1.236
1	16.45	2.71	6	26.2	1.741	1	38.85	1.225
1	17.0	2.63	1	26.85	1.702	1	39.6	1.206
½	18.2	2.46	3	27.4	1.670	1	40.5	1.184
½	19.0	2.36	½	28.5	1.611 } *b*	½	42.35	1.141*b*
8	19.7	2.28	1	28.85	1.593 }	1	43.05	1.126
1	20.1	2.24	½	30.15	1.531	2	44.35	1.100
6	20.9	2.15	2	31.1	1.488			

d doublet.
b broad.

from the Chancellor Mine, Boulder County, Colorado, gave identical *x*-ray powder patterns. The observed intensities, glancing angles, and measured spacings for these appear in Table 2.

JARLITE—$NaSr_3Al_3F_{16}$(?)

Jarlite, first described by Bøgvad (1933), occurs as colorless, flat crystals about 1 mm. in size, often fused in the shape of a fan and growing with thomsenolite in vugs in the cryolite. In the same paper Bøgvad described another new mineral occurring as grayish fan-shaped masses intergrown with chiolite. The two new minerals were found to have fairly similar optical properties and specific gravities, and chemical analyses of both, by Blix (in Bøgvad, 1933), led to the same ideal formula, $NaSr_3Al_3F_{16}$. Bøgvad considered the second mineral sufficiently different from jarlite to warrant a separate name, meta-jarlite.

In the present investigation, single-crystal photographs were taken of jarlite, and the powder photographs, optical constants, and specific gravities of both minerals were re-examined in order to clarify the relationship between them.

X-Ray Crystallography. From goniometric observations on crystals of typically poor development, Bøgvad showed that jarlite is monoclinic with tabular development parallel to the symmetry axis (Y optic direction) and a tendency towards elongation along this axis. Bøgvad found several faces besides the two opposite ones giving the tabular development, but the author could find only the latter on nearly a dozen crystals examined. For this reason, single-crystal orientation about the symmetry axis was possible only by adjusting in one plane, that normal to the faces, by the usual goniometric method, and in another plane, that containing the faces, by using the optical extinction direction in that plane. This method was applied with success to one jarlite crystal of which rotation, zero- and first-layer Weissenberg photographs were taken with unfiltered Cu radiation. These led to the possible space-groups $C2/m$, $C2$, Cm and, with the tabular faces basal, the cell dimensions, $a=15.99$, $b=10.82$, $c=7.24$, all ± 0.02 kX; $\beta=101°49'\pm 20'$. Only after this work had been completed was it discovered that the cell dimensions of jarlite had been determined earlier by Brosset (1942) who obtained $a=15.99$, $b=10.89$, $c=7.25$ Å, $\beta=78.2°$ (101.8°). The later independently determined values amply confirm the accuracy of Brosset's cell dimensions. The *x*-ray powder data for jarlite indexed to $\theta(\text{Cu})=25.1°$ on the new cell dimensions are given in Table 3.

Since meta-jarlite lacks crystal form, no attempt was made to examine it by single-crystal *x*-ray photographs; however, a powder photograph was taken and the observed data for it are given in comparison with those for jarlite in Table 3. Brosset (1942) published no powder data for the two minerals, but he does note that the two give generally similar powder patterns with line positions somewhat unlike but intensities largely in agreement. From this he concludes that the two minerals are likely isomorphous. The comparison in Table 3 verifies Brosset's observation that the two patterns are generally similar; spacings are slightly but consistently smaller for meta-jarlite, and there are some marked discrepancies in the intensities of corresponding lines. The differences, however, are not sufficiently great to alter Brosset's conclusion that the two minerals are probably isomorphous and indeed, meta-jarlite should probably be considered simply a variety of jarlite. This conclusion is strengthened by the similarity in other physical properties, notably the optical constants, of the two minerals as described below.

Geometrical Crystallography. An attempt was made to relate Bøgvad's morphological setting to the structural cell. Choosing the Y optic direction as $b[010]$ and the prominent tabular form as {100}, Bøgvad derived the following axial elements from the measurement of several faces on crystals of admittedly poor development: $a:b:c=1.46:1:2.58$, $\beta=69°\,20'$ (110° 40′). Since, as noted above, the tabular faces alone could be detected on the crystals used in the present investigation, the only direct evidence for relating the two settings is the coincidence of $b[010]$ in both (from the optics), and the equivalence of morphological {100} with structural {001}. With this limited information, the only method of relating the two settings completely is to derive, within the prescribed limitations, all reasonable transformations, calculate some of Bøgvad's observed interfacial angles for each transformation using the x-ray elements, and judge from the agreement between calculated and observed values which transformation is most probable. With this procedure, several possible transformations were derived of which the following appears to be the most likely:

Bøgvad to Ferguson: $00\bar{4}/060/301$

Applying this, Bøgvad's forms {100}, {010}, {001}, {110}, $\{\bar{1}01\}$ become respectively {001}, {010}, $\{\bar{4}01\}$, {021}, {201} in the structural setting. Due to the bad development of the crystals, agreement between the transformed morphological elements and the x-ray elements is very poor:

	a		b		c	β
Goniometric (Bøgvad)	1.72	:	1	:	0.704	104° 10′
X-ray (Ferguson)	1.478	:	1	:	0.669	101° 49′

Following is a comparison of Bøgvad's measured angles with those calculated from the new x-ray elements using the above transformation:

TABLE 3. JARLITE AND META-JARLITE: X-RAY POWDER PATTERNS

Jarlite Monoclinic, $C2/m$ $a=15.99$, $b=10.82$, $c=7.24$ kX, $\beta=101°\ 49'$					Meta-Jarlite		
I	θ(Cu)	d(meas.)	(hkl)	d(calc.)	I	θ(Cu)	d(meas.)
1	7.45°	5.93	$(\bar{2}01)$	5.888	2	7.55°	5.85
—	—	—	—	—	½	9.45	4.68
½	10.2	4.34	(021)	4.301	1	10.3	4.30
½	11.25	3.94	(400)	3.913	½	11.5	3.86
4	12.25	3.62	(311)	3.621	6	12.35	3.59
4	12.9	3.44	$(\bar{1}12)$	3.434	6	12.85	3.46
9	14.0	3.18	(420) (401)	3.170 3.613	9	14.2	3.13
6	14.35	3.10	$(\bar{3}12)$ $(\bar{4}21)$	3.120 3.092	7	14.5	3.07
10	15.0	2.97	(202) $(\bar{5}11)$ (022)	3.010 2.987 2.965	10	15.1	2.95
½	15.6	2.86	$(\bar{3}31)$	2.858	1	15.65	2.85
½	16.5	2.71	(421) (040)	2.730 2.705	2	16.6	2.69
½	17.0	2.63	$(\bar{6}01)$ (222)	2.629 2.628	1	17.1	2.61
—	—	—	—	—	1	17.75	2.52
3	19.05	2.36	$(\bar{6}21)$ (530) (003) $(\bar{1}13)$	2.364 2.364 2.363 2.353	2	19.1°	2.35
—	—	—	—	—	1	19.3	2.33
3	20.2	2.23	$(\bar{4}03)$ (440)	2.236 2.225	1	20.25	2.22
3	20.4	2.21	(113)	2.221	5	20.5	2.20
7	20.9	2.15	(023) (332) $(\bar{6}22)$ (203)	2.166 2.155 2.150 2.144	8	21.05	2.14

TABLE 3—(*continued*)

Jarlite					Meta-Jarlite		
I	θ(Cu)	d(meas.)	(hkl)	d(calc.)	I	θ(Cu)	d(meas.)
½	21.9	2.06	$(\bar{4}23)$ $(\bar{5}13)$	2.066 2.066	—	—	—
4	22.7	1.992	(350) $(\bar{8}01)$ (223) $(\bar{4}42)$ (711)	1.999 1.993 1.993 1.992 1.983	1	22.7	1.992
2	23.0	1.967	(313) $(\bar{6}03)$	1.971 1.963	7	23.05	1.963
—	—	—	—	—	1	23.5	1.928
—	—	—	—	—	1	24.25	1.872
1	24.35	1.864	(403)	1.861	2	24.45	1.857
6	25.1	1.812	$(\bar{5}33)$ (622) $(\bar{2}04)$	1.818 1.811 1.811	2	25.05	1.816

I	θ(Cu)	d(meas)	I	θ(Cu)	d(meas)
—	—	—	4	25.35°	1.795
2	25.55°	1.782	2	25.7	1.773
—	—	—	½	26.5	1.723
1	26.85	1.702	3	27.2	1.682
—	—	—	½	28.3	1.621
2	28.9	1.591	1	29.0	1.586
½	29.4	1.566	½	29.45	1.564
—	—	—	½	29.9	1.542
2	30.65	1.508	3	30.65	1.508
1	31.4	1.475	1	31.65	1.465
½	32.4	1.435	1	32.6	1.427
½	33.35	1.398	1	33.5	1.393
½	33.9	1.378	1	34.75	1.349
2	34.9	1.344	½	35.0	1.340
1	35.25	1.332	½	35.7	1.317
½	36.3	1.299	½	36.35	1.297
—	—	—	½	36.9	1.280
½	37.3	1.269	1	37.45	1.264
—	—	—	½	38.15	1.244
1	39.45	1.210	½	40.0	1.196
1	40.75	1.178	3	40.75	1.178
½	45.45	1.079	—	—	—
½	46.85	1.054	—	—	—
½	50.3	0.999	1	51.4	0.984

Morph. (Bøgvad)	Structural	Meas. (Bøgvad)	Calc. (Ferguson)
(100):(010)	(001):(010)	90° 00′	90° 00′
(100):(110)	(001):(021)	53 50	53 33½
(100):(001)	(001):$(\bar{4}01)$	69 20	70 25½
(100):$(\bar{1}01)$	(001):$(\bar{2}0\bar{1})$	33 30	36 45

Optics. Jarlite is biaxial positive or negative with $Y=b[010]$. A redetermination in sodium light of the indices of refraction by immersion gave values in close agreement with those of Bøgvad:

	α	β	γ
Bøgvad	1.427	1.432–1.433	1.435
Ferguson	1.430	1.435	1.437±0.002

For meta-jarlite, Bøgvad obtained an average value of 1.432±0.004. A complete new determination, also by immersion, gave $\alpha=1.429$, $\beta=1.431$, $\gamma=1.434$, all ±0.002. Since, as noted above, *x*-ray powder pictures suggest that meta-jarlite is only a variety of jarlite, the following average refractive indices appear the best for these two minerals when considered as one, jarlite:

$$\alpha=1.429,\ \beta=1.433,\ \gamma=1.436,\ \text{all } \pm 0.002$$

Using a universal stage and sodium light, Bøgvad measured $2V$ about X for six jarlite crystals, and obtained three angles from 78° 10′ to 80° 00′ (sign negative), and three others from 91° 40′ to 92° 30′ (sign positive). Three new measurements, also made on the universal stage, gave 81.1° (negative), 91.95° (positive), and 98.65° (positive). Since this angle varies so much, presumably with minor changes in chemical composition, a fair statement of the optic axial angle of jarlite is suggested as

$$2V=90°\pm 10°,\ \text{positive or negative}$$

No measurement of this angle has been made for meta-jarlite but, from the straightness of the brushes in the interference figure, it must be approximately 90° as indicated by Bøgvad. This observation is in keeping with the close similarity of meta-jarlite to jarlite in other respects.

Bøgvad established the following incomplete optic orientation of jarlite: $Y=b[010]$; optic axial plane $\perp$ $c(001)$ (structural setting); and $X{:}\perp c(001)=16°$ to 24° 15′. During the present study, these observations were checked and the complete optic orientation was established. For the angle $X{:}\perp c(001)$ Bøgvad obtained on three separate crystals the values 16°, 16°, 24° 15′. A re-measurement of this angle, also on three separate crystals each mounted for observation along [010] on the microscope stage, led to the values 16°, 17°, 19½° all ±1°. In order to determine the angle made by X with $c[001]$, it was necessary to use some method involving a single-crystal *x*-ray photograph since all crystals showed only the two basal faces. An attempt was made to mount a crystal for rotation about $c[001]$ using the known angles β and $X:\perp c(001)$ in conjunction with the goniometric reflection from a basal face, and assuming one of two possible orientations for $X:c[001]$, namely that X lies either in front of or behind c. With the latter orientation assumed, the first crystal mounted in this way gave a perfectly centered rotation photograph for a row whose period is 7.26 kX ($c[001]=7.24$ kX), thereby proving that this axis is $c[001]$ and that X lies *behind* $c[001]$. Thus, for an angle β 101° 49′ (say 102°) and for an angle $X:\perp c(001)$ of 17°, the orientation is $X:c[001] = -(17°-(102°-90°)) = -5°$. Or, considering the variation in $X:\perp c(001)$ as $16°-20°$, this orientation becomes $X:c[001] = -(4°-8°)$.

Composition, Cell Content, and Specific Gravity. It was noted above that chemical analyses of jarlite and meta-jarlite by Blix (in Bøgvad, 1933) led to the same ideal formula $NaSr_3Al_3F_{16}$ for both minerals. With Bøgvad's measured specific gravity of 3.93 and the author's cell dimensions, this formula gives a non-integral number of empirical formula weights in the unit cell ($Z \sim 4.4$). For $Z=4$, Bøgvad's ideal chemical formula gives a calculated density of 3.61. Of the various possible sources of error, the specific gravity seemed the most likely, and for this reason was carefully re-determined on three separate jarlite crystals using, as Bøgvad did, Clerici's solution and a Westphal balance. The three new values checked closely: 3.86_2, 3.86_4, 3.86_9 giving a new best value of 3.87 ± 0.01.

With the specific gravity now confirmed, and the correctness of the cell dimensions assured by the indexing of the powder photograph, the only possible conclusion is that the chemical formula, $NaSr_3Al_3F_{16}$, is in error. Once again, after this conclusion had been reached, it was found that Brosset (1942) had similarly reached the same conclusion some years earlier.

For meta-jarlite, Bøgvad measured the specific gravity as 3.78, using Clerici's solution. In the present study, relatively large fragments of meta-jarlite were available, and the specific gravity of two of these was measured on the Berman balance. These gave the values 3.59 (on 14 mg.) and 3.65 (on 24 mg.) indicating a minimum value, from the new measurements, of 3.65. The low value is attributed to the abundant inclusions which characterize specimens of meta-jarlite.

PROSOPITE—$CaAl_2(F,OH)_8$

This mineral has been reported from Ivigtut by Bøgvad (1938), who gives no descriptive details. Attempts to find prosopite again in the material available were unsuccessful; however, specimens from two of the well-established localities, Altenberg, Saxony, and St. Peter's Dome, El

Paso County, Colorado, were generously loaned by Professor Clifford Frondel of the Harvard Mineralogical Museum, and these made it possible to study this mineral.

The specimen from Saxony (Harvard 97155) showed relatively large (1 cm.) brownish-gray tabular crystals which proved, from an *x*-ray powder photograph, to consist of kaolinite, thus confirming the statements in the standard texts that prosopite from this locality is often largely altered to this mineral. The specimen from Colorado showed small (1 mm.), colorless, transparent, tabular crystals forming a druse on massive pachnolite. Both the morphological and the *x*-ray crystallography of these crystals has been studied by the staff at the Harvard labo-

TABLE 4. PROSOPITE—$CaAl_2(F, OH)_8$: *X*-RAY POWDER PATTERN

Monoclinic, *C*2/*c*; $a=6.67$, $b=11.17$, $c=7.37$ kX, $\beta=94°\ 56'$; $Z=4$

I	θ(Cu)	*d*(meas.)	(*hkl*)	*d*(calc.)	*I*	θ(Cu)	*d*(meas.)	(*hkl*)	*d*(calc.)
½	7.7°	5.74	(110)	5.711	4	20.3°	2.22	(042)	2.223
10	10.2	4.34	(111)	4.355	½	20.7	2.17	(310)	2.173
2	12.15	3.65	(002)	3.671	6	21.15	2.13	(240)	2.138
1	13.35	3.33	(200)	3.323				$(\bar{3}11)$	2.133
4	13.75	3.23	(130)	3.248	½	21.65	2.08	$(\bar{2}41)$	2.084
5	14.55	3.06	(022)	3.068	3	22.35	2.02	(241)	2.023
½	14.75	3.02	$(\bar{1}31)$	3.018				(151)	2.020
3	15.65	2.85	(220)	2.856	1	23.25	1.947	$(\bar{3}12)$	1.943
½	16.3	2.74	$(\bar{2}21)$	2.731	5	23.75	1.909	(133)	1.916
½	17.25	2.59	$(\bar{2}02)$	2.576				(330)	1.904
2	18.9	2.37	(202)	2.364	6	24.8	1.833	(004)	1.836
4	19.45	2.31	$(\bar{1}13)$	2.312	6	25.15	1.809	(331)	1.811

I	θ(Cu)	*d*(meas.)	*I*	θ(Cu)	*d*(meas.)	*I*	θ(Cu)	*d*(meas.)
½	26.15°	1.744	1	37.15°	1.273	½	49.75°	1.007
½	26.75	1.708	½	37.65	1.259	1	53.9	0.951
1	27.5	1.665	1	38.4	1.238	1	54.6	0.943
1	27.9	1.643	½	39.55	1.207	½	56.55	0.921
1	28.3	1.621	1	40.05	1.195	2	59.5	0.892
2	28.8	1.596	2	40.65	1.180	1	62.5	0.867
3	29.35	1.568	1	42.0	1.149	½	65.9	0.842
2	30.45	1.517	1	43.2	1.123	½	67.35	0.833
1	32.7	1.423	½	43.85	1.110	½	68.55	0.826
1	33.5	1.393	1	44.75	1.092	1	71.55	0.810
1	34.05	1.373	1	45.6	1.076	1	74.1	0.799
2	34.65	1.352	½	46.25	1.064	1	74.65	0.797
1	35.5	1.324	½	47.65	1.040	1	75.15	0.795
2	36.8	1.283	½	48.8	1.022			

ratory in connection with the preparation of Volume II of the Seventh Edition of Dana's *System of Mineralogy.* The present investigation was confined to verifying the cell dimensions and space-group previously determined at Harvard, and to establishing the indexed powder data.

Rotation and Weissenberg photographs were taken of two of the monoclinic crystals about axes [010] and [110]. These gave the monoclinic cell dimensions:

$$a=6.67,\ b=11.17,\ c=7.37,\ \text{all } \pm 0.02,\ \text{kX},\ \beta=94°\ 56'\pm 20'$$

which compare closely with the unpublished values derived at Harvard by Berman & Wolfe (private communication, 1941, kindly made available by Dr. Frondel):

$$a=6.69,\ b=11.11,\ c=7.32,\ \text{all } \pm 0.03\ \text{kX},\ \beta=95°\ 00'\pm 15'$$

The space-group was confirmed as *C2/c*. The powder data indexed to $\theta(\text{Cu})=25.15°$ on the author's cell dimensions, appear in Table 4. Certain small differences between these values and those given for prosopite from Saxony in the ASTM Card Index (1945, card 539), are probably due to small chemical difference in the material from two localities.

RALSTONITE—$Na_{2-x}(Al,Mg)_2(F,OH)_6\cdot 1-yH_2O$

Ralstonite occurs at Ivigtut with thomsenolite and cryolite as small, clear, colorless octahedral and cubo-octahedral crystals. For some time the chemical formula had been in doubt but Pabst (1939), in considering the structure of ralstonite, concluded that the best formula for the material from Ivigtut is $Na_{2.8}(Al,Mg)_{16}(F,OH)_{48}\cdot 7H_2O$. Since Pabst's work shows the structure to be defective with the 2.8 Na occupying a 16-fold position, and the $7H_2O$ occupying an 8-fold position in the space-group *Fd3m*, the formula could be written in the following way to indicate the defective nature of the structure: $Na_{16-x}(Al,Mg)_{16}(F, OH)_{48}\cdot 8-yH_2O$ with $x\sim 13$ and $y\sim 1$. In its simplest terms, this formula reduces to that given at the head of this section with $x\sim 1.6$ and $y\sim 0.1$.

Although earlier goniometric work and Pabst's later *x*-ray investigation indicated no departure from cubic symmetry, ralstonite has long been known to show "anomalous anisotropism." During the present study, one *x*-ray powder photograph of a good octahedral crystal gave a pattern which agreed well with Pabst's powder data, except that the new cell-edge, 9.92 kX, is noticeably larger than Pabst's, 9.87 Å. A second powder photograph of another ralstonite crystal, a cubo-octahedron, was similar to the first but showed one notable difference, namely that prac-

TABLE 5. RALSTONITE: COMPARISON OF OBSERVED *X*-RAY POWDER DATA

(*hkl*)	Pabst (Mo/Zr)		Ferguson (Cu/Ni)			
	(cubic)		(cubic)		(non-cubic)	
	I	*d*	*I*	*d*	*I*	*d*
(111)	10	5.68	10	5.70	10	5.77
(113)	8	2.97	9	2.99	9	2.99
(222)	7	2.84	8	2.86	8	2.86
(004)	1	—	1	2.47	1	2.47
(133)	2	2.26	3	2.27	3	2.27
(224)	4	2.01	4	2.03	4	2.02
(115) (333)	6	1.879	7	1.909	7	1.905
(044)	7	1.740	8	1.750	8	1.750
(135)	1	1.664	2	1.679	2	1.670
(026)	1	1.553	2	1.568	2	1.561
(335) (226)	4	1.485*b*	2	1.512	1	1.510
			5	1.497	4	1.495
(444)	1	1.421	1	1.435	½	1.429
(117) (155)	3	1.379	4	1.391	3	1.384*b*
(137) (355)	3	1.282	3	1.292	3	1.289
					3	1.283
(008)	1	1.228	1	1.240	1	1.239
					½	1.232
(228) (066)	2	1.158	3	1.171	3	1.167
					1	1.159
(266)	1	1.127	2	1.140	1	1.137
					½	1.129
(048)	1	1.102	1	1.111	1	1.109
					½	1.102
(119) (357)			½	1.090	½	1.084*b*
(466)			½	1.058	½	1.056*b*
(139)			1	1.042	½	1.039
					½	1.033
(448)			½	1.013	½	1.011*b*
			½	0.998	½	0.994
			½	0.974	½	0.972
			2	0.958	3	0.954*b*
			1	0.867	½	0.867
					½	0.861
			½	0.850	½	0.851
			2	0.842	1	0.841⎫*b*
			2	0.840	1	0.834⎭
			2	0.827	½	0.827
			1	0.818	½	0.819*b*
			½	0.805	½	0.812

b = broad band.

tically all lines beyond about $d=1.30$ kX appeared as doublets or as broadened bands. The extent of the broadening is shown in Table 5, which compares the observed data for the two new ralstonite photographs with those of Pabst.

In view of the optical anisotropism of the mineral, the most likely explanation for such broadening is a slight departure, in this crystal, from cubic symmetry. With this in mind, the author attempted to derive tetragonal (pseudo-cubic) cell dimensions from the powder photograph, but this proved unsuccessful. No further work was done on this crystal, and the only conclusion to be drawn from the line broadening is a suggestion of slight departure from cubic symmetry in that particular crystal of ralstonite.

X-ray powder photographs of four specimens of "hagemannite," a dull, yellow to brown ochre occurring with the cryolite and associated minerals at Ivigtut, confirmed the observation of Frondel (1948) that this "mineral" consists mainly of a variable mixture of ralstonite, thomsenolite, and goethite. The author's photographs indicated a predominance of ralstonite over thomsenolite in all four specimens.

WEBERITE—Na_2MgAlF_7

In 1938 Bøgvad described a new mineral from Ivigtut, weberite, which occurs as mottled-gray translucent masses with the cryolite, chiolite, topaz, etc. Bøgvad (1938) noted no crystals, but he did observe two cleavages, one prismatic and one pinakoidal, both poor. He also determined the specific gravity (2.96) and all the optical constants except the orientation. Brosset (1942) derived the orthorhombic cell dimensions and space-group, and Byström (1944) carried out a complete structure determination.

During the present investigation, the cell dimensions and space-group were re-determined, and the indices of the cleavage and optic orientation were established. Unsuccessful attempts were made to orient fragments for single-crystal photographs, using reflections from the uneven cleavage surfaces. Following this, an effort was made to orient an irregular fragment about one optical direction by adjusting the fragment, on the goniometer head, to extinction in two mutually perpendicular planes, on the stage of a petrographic microscope. For rotation about the *Z* optical direction, this gave good rotation and Weissenberg photographs, the rotation axis proving to be *c*[001] of Brosset. A second fragment was oriented in a similar manner for rotation about the *X* optical direction, the axis in this case proving to be *a*[100] of Brosset. The second fragment was not as well centered as the first, and the cell dimensions from it are considered less accurate. Following is a comparison of the cell dimen-

TABLE 6. WEBERITE—Na_2MgAlF_7: *X*-RAY POWDER PATTERN

Orthorhombic, *I2mm*; $a=7.29$, $b=7.05$, $c=9.97$ kX; $Z=4$

I	θ(Cu)	*d*(meas.)	(*hkl*)	*d*(calc.)
5	7.5°	5.89	(101)	5.885
6	8.75	5.05	(110)	5.068
3	12.5	3.55	(020)	3.525
½	14.65	3.04	(103)	3.024
9	15.1	2.95	(202)	2.942
9	15.45	2.89	(022)	2.878
½	17.6	2.54	(220)	2.534
4	18.9	2.37	(301)	2.361
5	19.5	2.30	(213)	2.319
4	20.05	2.24	(114)	2.237
			(130)	2.237
½	22.0	2.05	(204)	2.058
			(024)	2.035
3	23.0	1.967	(303)	1.962
			(321)	1.962
3	23.3°	1.943	(231)	1.937
1	24.9	1.826	(400)	1.823
10	25.6	1.779	(224)	1.777
1	26.9	1.699	(233)	1.698
1	27.5	1.665	(134)	1.665
			(006)	1.662
5	29.9	1.542	(305)	1.542
			(422)	1.540
4	30.5	1.515	(206)	1.512
			(242)	1.512
½	31.4	1.475	(404)	1.471
1	32.2	1.443	(501)	1.443
			(044)	1.439

I	θ(Cu)	*d*(meas.)
½	33.45°	1.395
1	35.05	1.339
1	37.2	1.271
½	38.0	1.249
½	38.6	1.232
½	39.35	1.212
½	40.6	1.181
½	41.35	1.164
3	42.0	1.149
½	42.9°	1.129
1	43.35	1.120
½	44.6	1.095
½	47.35	1.045
½	48.3	1.030
1	48.85	1.021
2	51.55	0.982
1	52.55	0.968
½	59.7	0.890
½	60.9°	0.880
½	62.0	0.871
2	63.75	0.857
3	64.6	0.851
3	65.3	0.846
2	67.3	0.833
1	71.5	0.811
2	73.6	0.801

sions of Brosset with the best of those derived from the two new sets of photographs:

	a	*b*	*c*
Brosset	7.29	7.05	9.97 Å
Ferguson	7.30	7.05	9.97 kX

The new values confirm Brosset's cell dimensions which are accepted for weberite in Table 6, giving the *x*-ray powder data indexed to θ(Cu) $=32.2°$.

Brosset's extinction conditions led to the possible space-groups *Immm*, *I*222, $I2_12_12_1$, *I2mm*, and Byström's structure is based on *I2mm*. Both investigators apparently observed only one weak exception to the condition (0*kl*) present only with $k=2n$ and $l=2n$, noting (0*kl*) present only with $(k+l)=2n$ and arriving at the above as possible space-groups. The author could detect no exceptions to the first condition on either set of Weissenberg photographs, and so deduced as possible space-groups *Ibmm* and *Ibm*2.

The optical character of the rotation axes of both fragments used for the x-ray photographs gave the optical orientation which is combined with the optical observations of Bøgvad as follows:

	(Na)	
$X=a[100]$	α 1.346	Positive
$Y=b[010]$	β 1.348	$2V=83°\pm 3°$
$Z=c[001]$	γ 1.350	

To determine the indices of the cleavage planes, a zero-layer Weissenberg photograph was taken about a random axis in the cleavage plane of one fragment. The various orders of reflection proved to be from planes (101), and thus the cleavage of weberite may be described as prismatic {101}, poor. The calculated acute cleavage angle $(101):(10\bar{1})$ about $c[001]=Z$, is 72° 21′ which is in excellent agreement with the acute cleavage angle about Z measured by Bøgvad in thin section, 72°. The second less conspicuous cleavage noted by Bøgvad as parallel to the optic axial plane would have indices {010}; this cleavage was not observed by the author.

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