THE RELATION OF LEIGHTONITE TO POLYHALITE

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The well-defined new mineral leightonite, described by Palache in the preceding communication, is especially interesting since it proves to be the copper homologue of the magnesium salt polyhalite. The chemical formulae of the two species compare as follows:

> Leightonite— $K_2Ca_2Cu(SO_4)_4 \cdot 2H_2O$ Polyhalite— $K_2Ca_2Mg(SO_4)_4 \cdot 2H_2O$

Homologous compounds are commonly homeomorphous. Both leightonite and polyhalite are triclinic, but in their present settings they do not show the expected geometrical similarity. In the natural pseudo-orthorhombic setting adopted by Palache, leightonite is developed prismatically with the axis c[001] and twinned on the sub-rectangular planes a(100) and b(010). For polyhalite Görgey (1915) chose a pseudo-monoclinic lattice:

$$a:b:c=0.9314:1:0.8562; \ \alpha=92^{\circ}29', \ \beta=123^{\circ}04', \ \gamma=88^{\circ}21'.$$

With reference to this lattice the crystals are commonly elongated with the axis a[100] and twinned on the sub-rectangular planes b(010) and c(001).

When polyhalite is turned forward about the normal to (010) until [100] comes into the vertical position the two crystal species agree in habit and twinning. Graphically the following planes come to near coincidence:

Polyhalite (Görgey)	Leightonite (Palache)
(100)	(101)
(010)	(010)
(001)	(100)
(212)	(111)

This correspondence gives the transformation:1

Görgey to Palache: $\frac{1}{2}01/010/\frac{1}{2}00$.

Applying the transformation to Görgey's elements we obtain the follow-

¹ The terms of the transformation formula are here written in the correct fractional form, as proposed by Dr. J. D. H. Donnay in a personal communication. In this form the transformation yields axial lengths and indices with the correct absolute values. If the transformation formula is cleared of fractions, as has always been done in the past, the resulting axial lengths and indices are proportional to the absolute values, which is adequate for morphological purposes if lattice centering is neglected.

ing elements of polyhalite which show the expected agreement with Palache's elements of leightonite:²

Polyhalitea:b:c:=0.7176:1:0.4657; $\alpha = 90^{\circ}39',$ $\beta = 90^{\circ}06\frac{1}{2}',$ $\gamma = 91^{\circ}53'$ Leightonitea:b:c=0.7043:1:0.4578; $\alpha = 90^{\circ},$ $\beta = 90^{\circ},$ $\gamma = 90^{\circ}$

The chemical similarity of the two species is thus accompanied by the usual similarity of form.

Table 1, computed by Mr. C. W. Wolfe, is an angle-table for the accepted forms of polyhalite, after Görgey, in Palache's setting. Comparing the form-symbols with those of Görgey (1915, p. 84) it will be found that an important simplification has been achieved.

Table 1. Polyhalite— $K_2Ca_2Mg(SO_4)_4 \cdot 2H_2O$

Triclinic; pinacoidal-T

	a:l	c = 0.7176	:1:0.4657;		$\alpha = 91^{\circ}$	°39′,	$\beta = 9$	$0^{\circ}06\frac{1}{2}'$,	$\gamma = 9$	1°53'		
	po: 90	$r_0 = 0.6490$:0.4660:1;	;	$\lambda = 88^{\circ}$	$20\frac{1}{2}'$	$\mu = 8$	39°501/2	,	$\nu = 8$	8°061/		
		Þ	0' = 0.6493	, 9	$_{0}'=0.4$	4661; a	$c_0' = 0$.0019,	3	$v_0' = 0$.0289		
Fo	rms	ϕ			ρ	1	4		1	В		4	С
b	010	0'	°00′	90°	°00′	88	$06\frac{1}{2}'$		0	°00′	8	8°	201/
a	100	88	$06\frac{1}{2}$	90	00	0	00		88	$06\frac{1}{2}$	8	9	50 ¹ / ₂
т	110	53	$05\frac{1}{2}$	90	00	35	01		53	$05\frac{1}{2}$	- 8	8	55
M	110	124	25 ¹ / ₂	90	00	36	19	1	24	251	9	0	51
0	$1\overline{2}0$	144	32	90	00	52	38 <u>±</u>	1	44	32	9	1	17
v	130	154	46	90	00	66	$39\frac{1}{2}$	1	54	46	9	1	27
w	140	160	36	90	00	72	291	1	60	36	9	1	31 1
γ	011	0	13	26	20	89	04	-	63	431	2	4	37
h	021	0	$06\frac{1}{2}$	43	52	88	37		46	08	4	2	$12\frac{1}{2}$
S	0T1	179	451	23	37	90	39 <u>1</u>	1	13	37	2	5	16
x	101	85	35	33	08	56	56		87	351	3	2	54
у	101	- 89	$19\frac{1}{2}$	32	$54\frac{1}{2}$	89	38		89	$50\frac{1}{2}$	3	3	02
e	111	51	341	39	43	59	$06\frac{1}{3}$		66	36	3	8	371
e	1 T 1	122	341	37	41	59	44	1	09	13	3	8	301
z	Ī11	- 53	$47\frac{1}{2}$	38	$43\frac{1}{2}$	119	$29\frac{1}{2}$		68	$18\frac{1}{2}$	3	7	51 <u>1</u>
u	111	- 125	19	38	25	121	$13\frac{1}{2}$	1	11	03	3	9	29
δ	131	24	$11\frac{1}{2}$	57	48	68	01		39	28 1	5	6	15
d	$1\overline{3}1$	154	$13\frac{1}{2}$	56	15불	70	191	1	38	29 1	5	7	42 1

² The details of the method of recomputing triclinic elements to a new setting by means of the transformation formula were recently given by Wolfe (1937).

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l	313	$-7551\frac{1}{2}$	33 43	$122 \ 14\frac{1}{2}$	$82\ 12\frac{1}{2}$	33 27
n	I 31	- 24 43	57 08	109 01	$40\ 16\frac{1}{2}$	$55 \ 40\frac{1}{2}$
t	T 51	- 15 28	67 36	$102 \ 32\frac{1}{2}$	$26 59\frac{1}{2}$	66 02
λ	313	$-102\ 51\frac{1}{2}$	$33 \ 34\frac{1}{2}$	122 53	97 05	34 05
ξ	212	$-109\ 12\frac{1}{2}$	34 25	$122 \ 39\frac{1}{2}$	100 43	35 06
ν	131	-155 03	56 54	$112 \ 13\frac{1}{2}$	139 25	58 27
au	151	-16426	$67\ 28\frac{1}{2}$	106 05	152 51	69 06
f	3T1	$100\ 50\frac{1}{2}$	63 15	29 25	99 $40\frac{1}{2}$	$63\ 28\frac{1}{2}$
g	331	123 49	$66\ 54\frac{1}{2}$	$41 \ 40\frac{1}{2}$	$120\ 47\frac{1}{2}$	67 45
i	5T1	95 49	72 58	18 39	95 33 ¹ / ₂	73 02

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The form series of polyhalite and leightonite, in the adopted pseudoorthorhombic setting, exhibit an interesting feature that indicates the nature of the structural lattices of the two species. This lies in the absence of forms which we would expect to be present if the chosen pseudoorthorhombic lattice were of the primitive mode. These absences show more clearly in polyhalite, which has the more fully developed formseries, and they are particularly evident in the gnomonic projection (Fig. 1) in which the radial lines are normals to the known vertical planes with symbols (hk0), the filled points are known planes with symbols (hk1), the blank points are known planes with symbols (hkl), where l is greater than 1. For the sake of simplicity and without introducing any significant error we may consider the lattice as orthorhombic and neglect the signs of the indices in the following consideration of lattice-plane spacings in relation to form development.

Whether we accept the Law of Bravais, or the Principle of Simplest Indices, such absences as (121), (141), are striking in view of the presence of (111), (131), (151); further, (221) is to be expected since (111), (331) are present; again (211), (411) should appear since (311), (511) are known.

These morphological absences are directly comparable to the familiar röntgenographic extinctions due to lattice centering, and they are interpreted in a similar manner. Lattice centering of the several possible types systematically halves the spacings of certain sets of planes in the simple lattice and thus doubles the corresponding indices (reciprocal lattice coordinates). Certain lattice planes (hkl) become ($2h \cdot 2k \cdot 2l$); (hkl) is extinguished as an x-ray diffraction spot, and the morphological importance of planes with the apparent symbol (hkl) is halved in keeping with the halved spacing, or reticular density, of the plane (Law of Bravais), and the increased complexity of the indices (Principle of Simplest Indices).

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FIG. 1. Polyhalite. Gnomonic projection of the known forms in the pseudo-orthorhombic setting (Table 1). The gnomonic net is the first layer |hk1| of the reciprocal lattice corresponding to the face-centered cell in the direct lattice (Fig. 3).



FIG. 2. Polyhalite. Gnomonic projection of the known forms in the normal setting. The gnomonic net is the first layer |kk1| of the reciprocal lattice corresponding to the simple cell in the direct lattice (Fig. 3).

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In the case of polyhalite the morphological absences indicate that the pseudo-orthorhombic lattice is an F-lattice in which all the faces of the primitive cell are centered. This type of centering results in halving the spacings of all planes whose indices in the primitive lattice do not conform to the law: h, k, l, all even, or h, k, l, all odd. It will be noticed that all the missing points mentioned above fail to conform to the F-lattice requirement, and thus we understand the failure of the corresponding planes to develop as crystal planes.

	Pseudo-orthorh	ombic - P	Pse	Pseudo-orthorhombic— F				
Forn	n <i>hkl</i>	d		Form	hkl	d		
b	010	4.29		b	020	2.25		
a	100	3.07		e e z(u)	111	1.55		
m M	110	2.48		a	200	1.54		
_	001	2.00		$\begin{pmatrix} m \\ M \end{pmatrix}$	220	1.24		
$\begin{pmatrix} \gamma \\ s \end{pmatrix}$	011	1.81		$\left \begin{array}{c} \delta \\ d \\ n \end{array} \right $	131	1.08		
0	120	1.75		-	002	1.00		
x) y)	101	1.67		$\begin{pmatrix} \gamma \\ s \end{pmatrix}$	022	0.91		
е е 2	111	1.55		f	311	0.89		
h	021	1.45		0	240	0.88		
	210	1.45		x y	202	0.84		
	121	1.31		g	331	0.76		
v	130	1.29		$t \\ \tau$	151	0.76		
-	201	1.21		h	042	0.73		

TABLE 2. POLYHALITE: INDICES AND SPACINGS

Table 2 gives the indices (hkl) and the relative spacings³ (d) of the thirteen planes with the greatest spacings in the primitive (P) lattice and in the face-centered (F) lattice. The important forms of polyhalite are, according to Görgey, $b \ a \ z \ y \ t \ M \ l \ o \ d \ n$, using the letters adopted in

³ Obtained by a graphical method which will be described elsewhere.

Table 1. The F-list clearly gives the better correspondence between morphological development and reticular spacings; and trials with the remaining possible modes of centering quickly show that they do not come into consideration.

Since the pseudo-orthorhombic lattice-cell of polyhalite is evidently face-centered and therefore a quadruple cell, we are confronted with the question: Would it not be proper to refer the morphology of polyhalite,



FIG. 3. Polyhalite. The direct lattice inferred from the morphology, showing the facecentered pseudo-orthorhombic cell (full lines) and the simple cell of the normal setting (broken lines).

and the homeomorphous species, leightonite, to a simple cell according to the principles of the normal triclinic setting recently proposed by the writer (1937) A, B) and adopted for the presentation of the morphology of several triclinic species? Figure 3 shows the lattice of polyhalite in which one pseudo-orthorhombic face-centered cell and one simple cell conforming to the requirements of the normal triclinic setting are outlined. The axes a', b', c', of the simple cell have the indices $[\frac{1}{2}0\frac{1}{2}], [0\frac{1}{2}\frac{1}{2}],$ $[00\overline{1}]$, with respect to the axes a, b, c, of the quadruple cell; consequently the transformation reads:

Pseudo-orthorhombic to Normal: $\frac{1}{2}0\frac{1}{2}/0\frac{1}{2}\frac{1}{2}/00\overline{1}$

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In the normal setting the forms of polyhalite appear as in Fig. 2, which may be compared with Fig. 1 giving the projection of the pseudoorthorhombic setting. The planes (100) and (010) and the axes [001] are parallel in the two settings; but since the vertical axes have opposite senses the one projection is the mirror image of the other. In the normal setting the basal plane slopes considerably to the front-right, and since the projection elements p_0' , q_0' are double the corresponding values in the pseudo-orthorhombic setting, the volume of the reciprocal lattice cell in the normal setting is four times the volume of the reciprocal lattice cells are in the converse relation. The normal setting gives some further simplification of indices since there are no systematic omissions.

The normal setting thus has certain advantages, and this setting should properly be adopted if absolute uniformity of treatment were the prime consideration. At the same time the normal setting would not reveal the remarkable pseudo-symmetry of the quadruple cell; and consequently the use of the pseudo-orthorhombic lattice is justified. The case is, in fact, exactly covered by the provision contained in the following statement (1937 A, p. 616):

The cases examined constitute a large proportion of the known triclinic minerals occurring in well-developed crystals, a sufficient number to warrant the conclusion that the normal setting, based on the smallest structure cell, is the proper setting for triclinic crystals except when well-marked pseudo-symmetry of habit points definitely to a simple multiple lattice of the structure lattice as the better morphological framework.

The structure lattices, it is true, have not been determined for the two minerals in question: the foregoing discussion rests wholly on morphological data in the light of the Law of Bravais. But in other cases similar considerations have led to the structural lattice. If a rigorous röntgenographic determination can be made, in spite of the difficulties which will arise from the complicated twinning, it will be interesting to compare the results with those obtained from the morphology.

SUMMARY

Leightonite— $K_2Ca_2Cu(SO_4)_4 \cdot 2H_2O$ is the copper homologue of polyhalite— $K_2Ca_2Mg(SO_4)_4 \cdot 2H_2O$. Suitably re-oriented polyhalite is similar to leightonite in its geometrical elements, habit and twinning. In the adopted orientation, in which an angle-table is given for polyhalite, the lattices of both species are triclinic with marked orthorhombic pseudo-symmetry. Morphological considerations indicate that this lattice is all-face-centered.

References

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