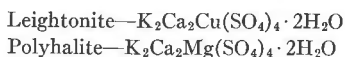


THE RELATION OF LEIGHTONITE TO POLYHALITE

M. A. PEACOCK, *University of Toronto, Toronto, Canada.*

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:



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)	(10 $\bar{1}$)
(010)	(010)
(001)	(100)
(2 $\bar{1}$ 2)	(111)

This correspondence gives the transformation:¹

$$\text{Görgey to Palache: } \frac{1}{2}01/010/\sqrt{\frac{3}{2}}00.$$

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

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

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— $\bar{1}$

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

$$p_0:q_0:r_0=0.6490:0.4660:1; \quad \lambda=88^{\circ}20\frac{1}{2}', \quad \mu=89^{\circ}50\frac{1}{2}', \quad \nu=88^{\circ}06\frac{1}{2}'$$

$$p_0'=0.6493, \quad q_0'=0.4661; \quad x_0'=0.0019, \quad y_0'=0.0289$$

Forms	ϕ	ρ	A	B	C
b 010	0°00'	90°00'	88°06½'	0°00'	88°20½'
a 100	88 06½	90 00	0 00	88 06½	89 50½
m 110	53 05½	90 00	35 01	53 05½	88 55
M 1 $\bar{1}$ 0	124 25½	90 00	36 19	124 25½	90 51
o 1 $\bar{2}$ 0	144 32	90 00	52 38½	144 32	91 17
v 1 $\bar{3}$ 0	154 46	90 00	66 39½	154 46	91 27
w 1 $\bar{4}$ 0	160 36	90 00	72 29½	160 36	91 31½
γ 011	0 13	26 20	89 04	63 43½	24 37
h 021	0 06½	43 52	88 37	46 08	42 12½
s 0 $\bar{1}$ 1	179 45½	23 37	90 39½	113 37	25 16
x 101	85 35	33 08	56 56	87 35½	32 54
y 1 $\bar{0}$ 1	— 89 19½	32 54½	89 38	89 50½	33 02
ϵ 111	51 34½	39 43	59 06½	66 36	38 37½
e 1 $\bar{1}$ 1	122 34½	37 41	59 44	109 13	38 30½
z 1 $\bar{1}$ 1	— 53 47½	38 43½	119 29½	68 18½	37 51½
u 1 $\bar{1}$ 1	— 125 19	38 25	121 13½	111 03	39 29
δ 131	24 11½	57 48	68 01	39 28½	56 15
d 1 $\bar{3}$ 1	154 13½	56 15½	70 19½	138 29½	57 42½

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).

<i>l</i>	$\bar{3}13$	— 75 $51\frac{1}{2}$	33 43	122 $14\frac{1}{2}$	82 $12\frac{1}{2}$	33 27
<i>n</i>	$\bar{1}31$	— 24 43	57 08	109 01	40 $16\frac{1}{2}$	55 $40\frac{1}{2}$
<i>t</i>	$\bar{1}51$	— 15 28	67 36	102 $32\frac{1}{2}$	26 $59\frac{1}{2}$	66 02
λ	$\bar{3}\bar{1}3$	—102 $51\frac{1}{2}$	33 $34\frac{1}{2}$	122 53	97 05	34 05
ξ	$\bar{2}12$	—109 $12\frac{1}{2}$	34 25	122 $39\frac{1}{2}$	100 43	35 06
ν	$\bar{1}\bar{3}1$	—155 03	56 54	112 $13\frac{1}{2}$	139 25	58 27
τ	$\bar{1}\bar{5}1$	—164 26	67 $28\frac{1}{2}$	106 05	152 51	69 06
<i>f</i>	$3\bar{1}1$	100 $50\frac{1}{2}$	63 15	29 25	99 $40\frac{1}{2}$	63 $28\frac{1}{2}$
<i>g</i>	$3\bar{3}1$	123 49	66 $54\frac{1}{2}$	41 $40\frac{1}{2}$	120 $47\frac{1}{2}$	67 45
<i>i</i>	$5\bar{1}1$	95 49	72 58	18 39	95 $33\frac{1}{2}$	73 02

The form series of polyhalite and leightonite, in the adopted pseudo-orthorhombic 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 pseudo-orthorhombic lattice were of the primitive mode. These absences show more clearly in polyhalite, which has the more fully developed form-series, 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).

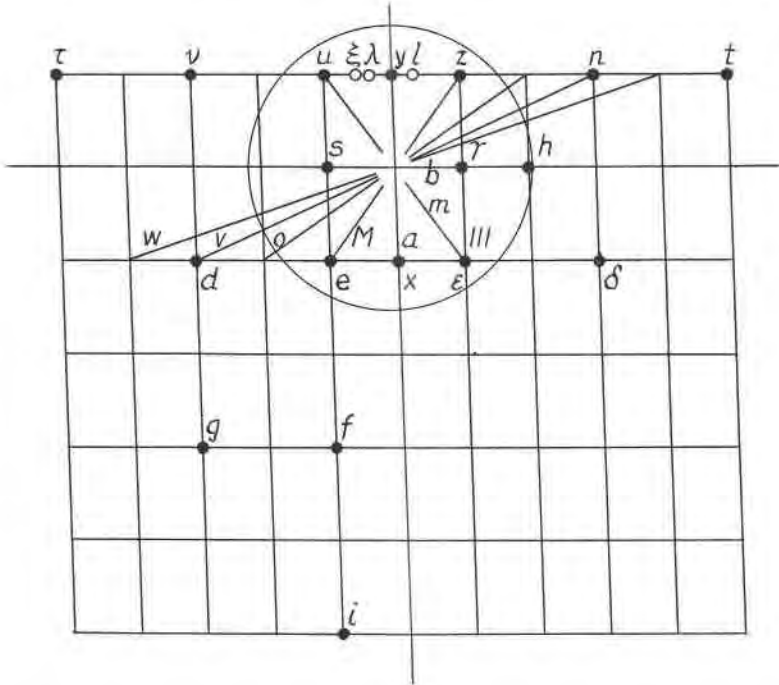


FIG. 1. Polyhalite. Gnomonic projection of the known forms in the pseudo-orthorhombic setting (Table 1). The gnomonic net is the first layer $|hk1|$ of the reciprocal lattice corresponding to the face-centered cell in the direct lattice (Fig. 3).

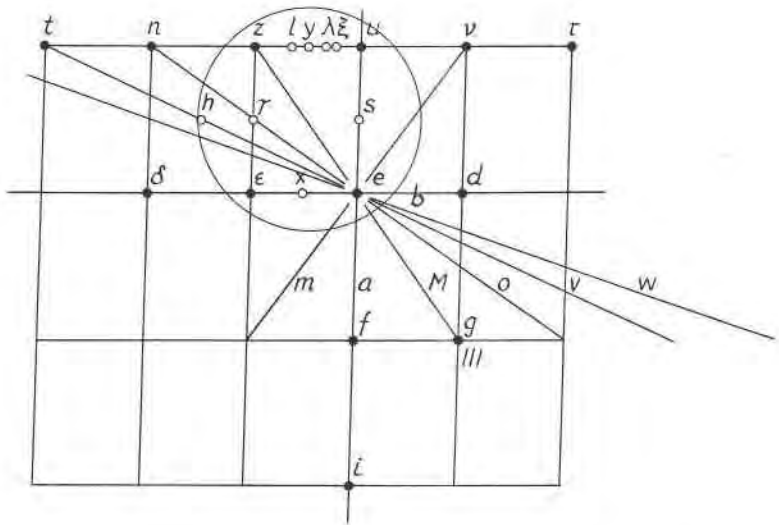


FIG. 2. Polyhalite. Gnomonic projection of the known forms in the normal setting. The gnomonic net is the first layer $|hk1|$ of the reciprocal lattice corresponding to the simple cell in the direct lattice (Fig. 3).

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.

TABLE 2. POLYHALITE: INDICES AND SPACINGS

Pseudo-orthorhombic— P			Pseudo-orthorhombic— F		
Form	hkl	d	Form	hkl	d
b	010	4.29	b	020	2.25
a	100	3.07	ϵ	111	1.55
			e		
z					
u					
m	110	2.48	a	200	1.54
M					
—	001	2.00	m	220	1.24
			M		
γ	011	1.81	δ	131	1.08
s					
d					
n					
v			ν		
o	120	1.75	—	002	1.00
x	101	1.67	γ	022	0.91
y					
s			s		
ϵ	111	1.55	f	311	0.89
e					
z					
u					
h	021	1.45	o	240	0.88
—	210	1.45	x	202	0.84
			y		
—	121	1.31	g	331	0.76
v	130	1.29	l	151	0.76
			τ		
—	201	1.21	h	042	0.73

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 G6rg6y, $b a z y t M l o d n$, 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,

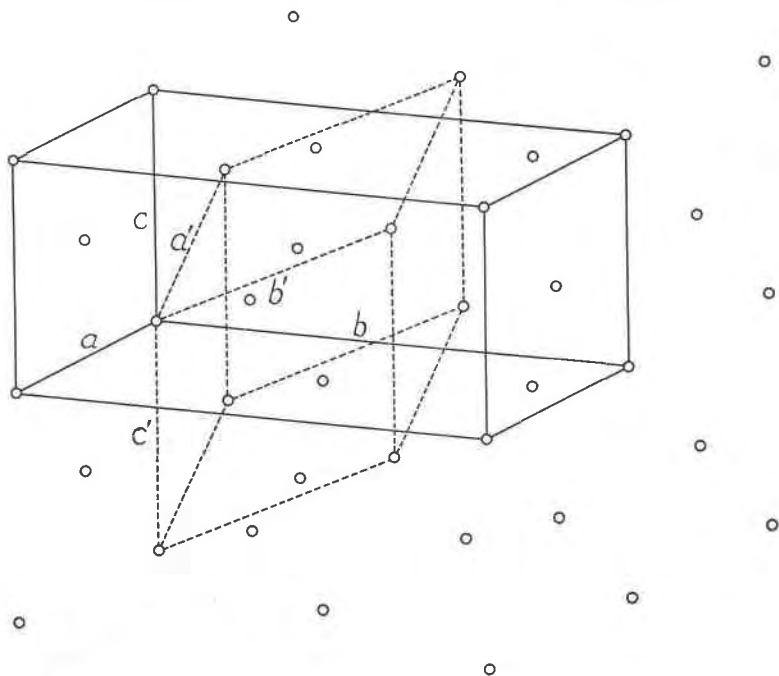


FIG. 3. Polyhalite. The direct lattice inferred from the morphology, showing the face-centered pseudo-orthorhombic cell (full lines) and the simple cell of the normal setting (broken lines).

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 $[\frac{1}{2}0\frac{1}{2}]$, $[0\frac{1}{2}\frac{1}{2}]$, $[00\bar{1}]$, with respect to the axes a , b , c , of the quadruple cell; consequently the transformation reads:

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

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 pseudo-orthorhombic 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 cell in the pseudo-orthorhombic setting. The volumes of the direct 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— $\text{K}_2\text{Ca}_2\text{Cu}(\text{SO}_4)_4 \cdot 2\text{H}_2\text{O}$ is the copper homologue of polyhalite— $\text{K}_2\text{Ca}_2\text{Mg}(\text{SO}_4)_4 \cdot 2\text{H}_2\text{O}$. 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

- GÖRGEY, R. (1915): Über die Krystallform des Polyhalit—*Min. Pet. Mitt.*, vol. **33**, pp. 48–102.
- PEACOCK, M. A. (1937 A): On the Crystallography of Axinite and the Normal Setting of Triclinic Crystals—*Am. Mineral.*, vol. **22**, pp. 588–624.
- (1937 B): The Normal Triclinic Setting: Correction—*Am. Mineral.*, vol. **22**, pp. 987–989.
- WOLFE, C. W. (1937): Re-orientation of Römerite—*Am. Mineral.*, vol. **22**, pp. 736–741.