

ON ROSELITE AND THE RULE OF HIGHEST PSEUDO-SYMMETRY

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SUMMARY

Revision of the geometrical and optical crystallography of roselite— $(\text{Ca}, \text{Co}, \text{Mg})_3\text{As}_2\text{O}_8 \cdot 2\text{H}_2\text{O}$ from Schneeberg, Saxony, leads to results that differ in many important respects from the classical data of Schrauf (1874). Roselite proves to be monoclinic, prismatic; $a:b:c=0.8780:1:0.4398$, $\beta=100^\circ 53'$; forms: $c\{001\}$, $b\{010\}$, $a\{100\}$, $j\{120\}$, $k\{350\}$, $l\{230\}$, $m\{110\}$, $n\{210\}$, $o\{012\}$, $p\{111\}$, $q\{\bar{1}11\}$, $r\{238\}$, $s\{\bar{1}22\}$, $t\{454\}$; cleavage $\{010\}$; twin plane (100). Pale rose crystals show: X (pale rose): $[001]=+0^\circ$ to 1° ; Y (paler rose) $= [010]$; Z (palest rose); indices (Na): $nX=1.694$, $nY=1.704$, $nZ=1.719$; positive; $2V=75^\circ$; $r < v$. Dark rose crystals are zoned; X (deep rose) $= [010]$; Y (pale rose): $[001]=+12^\circ$ to 20° ; Z (paler rose); indices (Na): $nX=1.725$, $nY=1.728$, $nZ=1.735$; positive; $2V=60^\circ$; $r < v$. As now described, roselite is homeomorphous with branditite— $\text{Ca}_2\text{MnAs}_2\text{O}_8 \cdot 2\text{H}_2\text{O}$, as described by Aminoff (1919).

Roselite is another case in which the lattice with the highest pseudo-symmetry (pseudo-orthorhombic) is a multiple lattice of the proper crystal lattice. In all such cases the Rule of Highest Pseudo-Symmetry gives unsatisfactory morphological elements and abnormal form symbols.

Pseudo-symmetry is one of the most remarkable facts of crystallography. With axial angles approaching 90° or 60° and axial lengths nearing equality, many crystal species of low real symmetry simulate higher symmetry in their geometrical elements. This metrical¹ pseudo-symmetry of the morphological lattice is typically accompanied by corresponding pseudo-symmetry in the arrangement and development of the forms, in the geometry of the diffraction patterns obtained with x -rays, and in the optical behaviour. Furthermore, since planes and axes of pseudo-symmetry are commonly planes and axes of twinning, crystals with pseudo-symmetrical lattices frequently occur in twinned complexes actually possessing the elements of symmetry of the higher system simulated by the homogeneous crystal. By pseudo-symmetry the properties of a crystal may approach those of any higher system. Examples of all the possible cases of pseudo-symmetry are known, even of the extreme case of triclinic crystals that approach the symmetry of the cubic system.

In pseudo-symmetrical crystals the geometrical constants may depart from the simulated higher symmetry by amounts which cannot be overlooked, say one degree or more in axial angle or one per cent or more in axial length. In many cases, however, the departures are much smaller and pseudo-symmetry has been detected and demonstrated only by close study of favourable material. Finally, there are cases in which

¹ The use of "metrical" in this sense was suggested to me in conversation by Professor R. L. Parker, in Zürich.

pseudo-symmetry is justly suspected, but cannot be proved by goniometry since the metrical departure from higher symmetry is less than the probable error of observation.

The fundamental nature of pseudo-symmetry has been recognized by most morphologists, and what may be called the Rule of Highest Pseudo-Symmetry has been widely applied in selecting crystallographic elements. By this rule the lattice with the highest pseudo-symmetry is chosen and oriented in the manner proper to the system approached by the pseudo-symmetrical crystal. Frequently this procedure has led to elements exhibiting true pseudo-symmetry of the species; but in some cases the quality of pseudo-symmetry has been strained, as shown by unnatural form symbols and lack of pseudo-symmetry beyond the metrical pseudo-symmetry of the chosen lattice. Friedel (1904) has discussed many striking cases of the misuse of the principle of pseudo-symmetry in determining crystallographic elements. A further example is provided by roselite, in which the presumed pseudo-symmetry led not only to unnatural form symbols but, as it now appears, to the acceptance of fictitious forms. Furthermore, a re-study shows that a too serious regard to small angular differences has resulted in roselite being placed in the wrong crystal system and provided with a series of twin laws, of which some are certainly imaginary.

SYMMETRY, ELEMENTS, FORMS

Roselite, the rose-red arsenate of lime and cobalt, was named by Lévy (1824), who described the crystals as orthorhombic. This interpretation was accepted until Schrauf (1873, 1874) concluded, from detailed studies, that roselite has pseudo-orthorhombic triclinic elements, and that the crystals are lamellar complexes twinned on as many as five of the six elements of pseudo-symmetry of the chosen lattice. While there is nothing inherently unlikely in this conception, Schrauf's form symbols indicate a false choice of morphological lattice. In his notation the vertical zone contains only one certain form, the eminent cleavage $\{100\}$; such simple forms as $\{010\}$, $\{120\}$, $\{\bar{1}20\}$, $\{011\}$, $\{0\bar{1}1\}$, $\{101\}$, $\{\bar{1}01\}$, were not observed, although they are entered as hypothetical forms in the angle-table and projection; and the main zone has the improbable symbol series: $\{\bar{1}00\}$, $\{803\}$, $\{201\}$, $\{\bar{4}03\}$, $\{\bar{2}03\}$, $\{203\}$, $\{403\}$, $\{201\}$, $\{803\}$, $\{100\}$.

In a review of Schrauf's work Dr. Laurence LaForge observed these abnormalities and found that by taking Schrauf's (041) as the axial plane (010), retaining Schrauf's (100), (001), (111) with their symbols unchanged, many of the forms received normal symbols while the remainder, if slightly displaced, could be explained by twinning. Although such

an interpretation was supported by the appearance of some of Schrauf's figured crystals, a re-investigation was necessary to test and give precision to LaForge's promising supposition and to clear up remaining uncertainties in the morphology and optics of the species.

The crystals studied were detached from two specimens from the Karabacek collection, recently acquired by the Harvard Mineralogical Museum. The specimens come from Schneeberg in Saxony, where rose-lite has been found on two occasions, first in the Rappold mine, about 1800 or earlier, and again in 1873, in the Daniel mine. One specimen (H. M. M. 93835) carries light-rose crystals whose appearance and association agree exactly with Schrauf's description of the material from the Daniel mine; the other (H. M. M. 93836) has cavities largely filled with deep-rose interlocking crystals corresponding precisely with the Rappold material. Morphologically the two varieties cannot be distinguished, although, as will appear later, they exhibit marked optical differences corresponding to differences in composition and specific gravity, recorded by Schrauf.

The crystals suitable for goniometric study measure less than 1 mm. in greatest dimension. They possess only one highly developed zone, taken as [010] by Schrauf, which contains the single eminent cleavage, {100} of Schrauf. The main zone is properly taken as the vertical zone [001], with the cleavage as {010}; this is the position adopted by Goldschmidt (1897), and considerations of symmetry will show that it is the only reasonable position for the mineral.

The habit is stout prismatic, or rarely thick-tabular after the plane taken as (001), with simple terminations of monoclinic or orthorhombic aspect. Only the smallest crystals have faces giving single sharp reflections; most of the faces give double or multiple reflections in somewhat varying positions, evidently due to the zoned structure of the crystals, later determined optically. These multiple reflections prevent very precise measurement, and they result in a range in the measured angles for the several forms which is wider than usual.

It soon appeared that the morphological lattice of roselite is not pseudo-orthorhombic, as Schrauf believed, but pseudo-monoclinic or truly monoclinic, with a pronounced inclination of the fore-and-aft axis to the vertical. With such a lattice the principal terminal planes, (041), (111), ($\bar{1}11$), ($\bar{2}2\bar{1}$), ($22\bar{1}$), in Schrauf's notation, become (001), (111), ($\bar{1}\bar{1}1$), ($\bar{1}\bar{1}1$), ($\bar{1}11$), respectively, perfectly normal and ideally simple symbols. It was also found that the crystals are, almost without exception, twinned by reflection in (100), which causes the pseudo-orthorhombic appearance of most of the terminations. These findings completely confirmed LaForge's supposition based on a consideration of Schrauf's unnatural indices.

A discussion of the best measurements at first led to triclinic elements with the axial angles: $\alpha = 90^\circ 07\frac{1}{2}'$, $\beta = 100^\circ 41'$, $\gamma = 90^\circ 39'$. As far as the measurements showed α might have been exactly 90° ; on the other hand, it seemed that γ was certainly not a right angle since (010) was repeatedly observed to be inclined to (010) twinned by reflection in (100) at the considerable average angle of $1^\circ 18'$ (mean of six measurements). After the morphology was completed on this basis, the preparation of cleavage plates for optical study revealed a remarkable fact: the cleavages (010) and (010) twinned by reflection in (100) gave a perfectly coplanar surface on a twin crystal which showed a definite re-entrant between the corresponding faces. The test was repeated on another twin, with the same result. This showed beyond dispute that (010) and (100) make exactly a right angle; and therefore, since the angle from (010) to (001) is also sensibly 90° , roselite is not triclinic with pseudo-monoclinic symmetry but truly monoclinic. The lack of exact parallelism between the cleavage surface and the external face may be explained by disturbance due to zonal growth, and consequently the slight departure of other faces from exact monoclinic relation is not significant. The similarity of faces on either side of (010), and of upper and lower terminations brought into symmetrical juxtaposition by twinning on (100), show that roselite belongs to the holohedral or prismatic class ($2/m$) of the monoclinic system.

Since roselite proves to be monoclinic, with the cleavage as the symmetry plane, the adopted setting with the main zone vertical and the cleavage as {010} is correct. As the five most important terminal planes give simplest indices, the base is properly chosen. In regard to the choice of parametral plane there are two possibilities: either we take the unknown form {212} as the unit positive pyramid, giving $n\{110\}$, $m\{120\}$, $l\{130\}$, $k\{3.10.0\}$, $j\{140\}$, as the vertical prism series; or we accept the only important positive pyramid p as {111}, giving $n\{210\}$, $m\{110\}$, $l\{230\}$, $k\{350\}$, $j\{120\}$ in the vertical zone. Although the author is inclined to believe that the first alternative would give the translation lattice, the morphology seems to demand the second choice, which is adopted.

The mean measured angles on the forms $m\{110\}$, $n\{210\}$, $p\{111\}$, which have faces much superior to those of the remaining forms, give the following projection elements:

$$p_0' = 0.5101, q_0' = 0.4398; x_0' = 0.1923$$

yielding polar and linear elements which define the morphological lattice of roselite with fair precision:

$$p_0 : q_0 : r_0 = 0.5009 : 0.4319 : 1; \mu = 79^\circ 07'$$

$$a : b : c = 0.8780 : 1 : 0.4398; \beta = 100^\circ 53'$$

Two-circle measurements on ten crystals, all but one of which are twins, are summarized in Table 1. Although the measurements range rather widely, for the reason already given, the mean observed angles agree satisfactorily with the calculated values.

TABLE 1. ROSELITE. MEASURED AND CALCULATED, TWO-CIRCLE ANGLES
 $\phi_0' = 0.5101$, $q_0' = 0.4398$; $x_0' = 0.1923$

Forms	Faces	Measured Range		Measured Mean		Calculated	
		ϕ	ρ	ϕ	ρ	ϕ	ρ
<i>c</i> {001}	10	87°53'–93°23'	10°15'–12°30'	89°34'	11°06'	90°00'	10°53'
<i>b</i> {010}	18	— 0 55 – 1 00	—	— 0 07	90 00	0 00	90 00
<i>a</i> {100}	7	89 18 –90 34	—	89 56	90 00	90 00	90 00
<i>j</i> {120}	17	29 35 –31 44	—	30 53	90 00	30 06½	90 00
* <i>k</i> {350}	11	34 16 –35 24	—	34 45	90 00	34 50	90 00
<i>l</i> {230}	15	36 50 –38 14	—	37 32	90 00	37 42½	90 00
<i>m</i> {110}	11	48 50 –49 36	—	49 14	90 00	49 14	90 00
<i>n</i> {210}	23	66 21 –67 10	—	66 42	90 00	66 41	90 00
<i>p</i> {111}	24	57 16 –58 25	39 20 –40 04	57 57	39 39	57 57	39 39
<i>q</i> {1̄11}	8	–35 04 –37 18	28 00 –28 37	–36 10	28 15	–35 51	28 29
* <i>r</i> {238}	4	20 08 –20 39	10 07 –10 31	20 27	10 15	21 27	10 03
* <i>s</i> {1̄22}	4	—	—	– 7	25	– 8 07	23 57
* <i>t</i> {454}	4	51 53 –52 18	41 25 –41 44	52 07	41 38	51 57	41 44

* New form.

The forms observed on roselite have the following characteristics:

c{001}: common; usually small, sometimes absent; rarely large producing a thick tabular habit; surface dull giving a weak reflection.

b{010}: cleavage; present as a face on all crystals; generally narrow; surface and reflection fairly good.

a{100}: common; usually narrow, sometimes absent; rarely broad; striated with [001]; surface and reflection fair.

j{120}, *k*{350}, *l*{230}: all common, usually occurring together in a somewhat curved and striated part of the prism zone; the three simple rational symbols represent positions in which the somewhat scattered reflections in this region congregate.

m{110}: common; medium to narrow; surface and reflection very good.

n{210}: present on all crystals; generally broad; surface and reflection very good.

p{111}: present on all crystals; large; surface and reflection very good, sometimes excellent.

- $q\{\bar{1}1\}$: fairly common; smaller than p ; surface and reflection poor.
 $r\{\bar{2}38\}$: four faces on one twin; small, surface poor; reflection weak.
 $s\{\bar{1}22\}$: uncommon but large; surface uneven; reflection blurred; symbol determined graphically; the form would not be retained if it did not produce important modification in the appearance of some crystals.
 $t\{454\}$: four faces on one twin; narrow; surface fair; reflection weak.

Table 2 is a formal angle-table for the accepted forms of roselite; Fig. 1 gives the corresponding stereographic projection.

TABLE 2. ROSELITE—(Ca, Co, Mg)₃As₂O₈·2H₂O

Monoclinic; prismatic— $2/m$
 $a : b : c = 0.8780 : 1 : 0.4398$; $\beta = 100^\circ 53'$
 $p_0 : q_0 : r_0 = 0.5009 : 0.4319 : 1$; $\mu = 79^\circ 07'$
 $r_2 : p_2 : q_2 = 2.3155 : 1.1599 : 1$;
 $p_0' = 0.5101$, $q_0' = 0.4398$; $x_0' = 0.1923$

Forms	ϕ	ρ	ϕ_2	$\rho_2=B$	C	A
c 001	90°00'	10°53'	79°07'	90°00'	0°00'	79°07'
b 010	0 00	90 00	—	0 00	90 00	90 00
a 100	90 00	90 00	0 00	90 00	79 07	0 00
j 120	30 06½	90 00	0 00	30 06½	84 34	59 53½
k 350	34 50	90 00	0 00	34 50	83 48½	55 10
l 230	37 42½	90 00	0 00	37 42½	83 22	52 17½
m 110	49 14	90 00	0 00	49 14	81 46½	40 46
n 210	66 41	90 00	0 00	66 41	80 01	23 19
o 012	41 10	16 17	79 07	77 49	12 11	79 22
p 111	57 57	39 39	54 55	70 12½	30 53	57 15½
q $\bar{1}11$	—35 51	28 29	107 38	67 15½	35 52	106 13
r $\bar{2}38$	21 27	10 03	86 17½	80 39	11 46	86 20½
s $\bar{1}22$	— 8 07	23 57	93 35½	66 18	27 23	93 17½
t 454	51 57	41 44	54 55	65 46½	33 42½	58 23½

TWINNING

Single crystals of roselite (Fig. 2) are very rare; nearly all the crystals are twinned by reflection in (100) which is also the plane composition surface separating a pair of symmetrical individuals (Figs. 3–6). In most cases the trace of the plane of twinning and composition can be seen on (010) and followed in more or less well-marked re-entrants between the two terminations. Occasionally the twin junction is not visible, but it can always be verified optically in cleavage plates traversing the entire crystal. In one case (Fig. 5) twinning has resulted in a fourling of Roc

tourné type, in which the diagonally opposite parts are in parallel position, while adjacent parts in contact on (110) are twinned by reflection in this plane.

The following angles, on a small exceptionally good crystal selected and measured by Professor Palache, show how accurately the terminations are symmetrical about the trace of (100):

	MEASURED		CALCULATED	
	ϕ	ρ	ϕ	ρ
$p(111)$	58°12'	39°35'	57°57'	39°39'
$p(111)$ twin	- 58 14	39 35	- 57 57	39 39
$p(1\bar{1}1)$	122 02	39 35	122 03	39 39
$p(1\bar{1}1)$ twin	-122 02	39 35	-122 03	39 39

In terms of Friedel's excellent development of the treatment of twinning of the French School (1926, pp. 421-483; 245-252) the present twin law is a case of twinning by reticular pseudo-merohedry with index 3 and obliquity $1^{\circ}16\frac{1}{2}'$. The twin plane (100) (Fig. 7) is a plane of pseudo-symmetry, not of the monoclinic crystal lattice $ABCD$, but of the pseudo-orthorhombic simple multiple lattice $EBFD$ —the twin lattice—which can be reflected in (100) with only small deviation at the twin junction (twinning by reticular pseudo-merohedry). The twin lattice restores one third of the total number of lattice points (index 3), and the normal to the twin plane (100) is inclined to the lattice row [301], which is quasi-normal to the twin plane, at $1^{\circ}16\frac{1}{2}'$ (obliquity). According to the French theory the twin growth occurs in this case because the crystal lattice fortuitously possesses a simple multiple lattice with small index and obliquity.

The twin law described above is equivalent to Schrauf's law (β), which he defined as a rotation of 180° about the normal to $C(001) = a(100)$ of our setting; for Schrauf's remaining laws (α), (γ), (δ), (ϵ), (ζ), (η), we can find no morphological or optical evidence. Of these laws, (α), equivalent to reflection in (010), and (γ), 180° rotation about [010], must be excluded since (010) and [010] are symmetry elements in the prismatic class of the monoclinic system. On the other hand, Schrauf's laws (ζ), 180° rotation about [001], and (η), 180° rotation about [301], and reflection in ($\bar{1}03$), which is not mentioned by Schrauf, are probable twin laws since [001], [301], ($\bar{1}03$), together with (100), are the four elements of pseudo-symmetry of the twin lattice $EBFD$ (Fig. 7). Schrauf's remaining laws, (δ), (ϵ), are compound laws involving no new twinning element. The confirmed law and the three probable laws constitute a group of "correspondent twins" (*macles correspondantes* of Friedel) due to the pseudo-symmetry of one and the same lattice.

CORRELATION

The new observations may be compared with those of Schrauf by means of Goldschmidt's two-circle angles computed from Schrauf's data in the position which we have adopted. Table 3 compares our range of measured angles for three typical forms with those of Goldschmidt (1897) after Schrauf. Although the agreement is only tolerable, due to the imperfection of the material and the many peculiar difficulties of the case, the table shows the nature of the correlation between our forms and those of Schrauf. Due to the monoclinic symmetry, each of our forms $\{hkl\}$ is equivalent to two of Schrauf's forms, while the monoclinic symmetry together with the twinning on (100) makes each of our general forms $\{hkl\}$ equivalent to four of Schrauf's forms.

TABLE 3. ROSELITE. COMPARISON OF ANGLES

	Measured Range		Goldschmidt after Schrauf		
	ϕ	ρ		ϕ	ρ
$m \begin{cases} 110 \\ \bar{1}\bar{1}0 \end{cases}$	48°50' - 49°36'	90°00'	ϕ 320	49°05'	90°00'
	131 10 -130 24	90 00	f $3\bar{2}0$	131 34	90 00
$n \begin{cases} 210 \\ 2\bar{1}0 \end{cases}$	66 21 - 67 10	90 00	η 310	66 49	90 00
	113 39 -112 50	90 00	e $3\bar{1}0$	114 09½	90 00
$p \begin{cases} 111 \\ \bar{1}\bar{1}\bar{1} \\ 111 \text{ tw.} \\ \bar{1}\bar{1}\bar{1} \text{ tw.} \end{cases}$	57 16 - 58 25	39 20 -40°04'	S 212	57 04	40 11½
	122 44 -121 35	39 20 -40 04	σ $2\bar{1}\bar{2}$	122 24	40 01½
	- 57 16 - 58 25	39 20 -40 04	s $2\bar{1}2$	- 54 55	39 28½
	-122 44 -121 35	39 20 -40 04	Σ $2\bar{1}\bar{2}$	-122 54½	38 45½

A full correlation of the form-letters and symbols of Schrauf, Dana, Goldschmidt and the author are given in table 4. The transformation formulas² cannot, of course, take account of twinning, and therefore they necessarily give two true symbols, and two false symbols for each (hkl) plane in twin position. In Schrauf's column the form letters in parentheses are the hypothetical forms, most of which were accepted by Dana but were properly neglected by Goldschmidt. The last column shows the accepted forms of roselite. Schrauf's hypothetical forms are neglected, none of them having been found in the present study; the rest have been transformed to the new lattice, those provided with letters being accepted, those marked with a dash rejected. Schrauf's m M are founded on single doubtful observations; the planes lie in the vicinity of our $s \{ \bar{1}22 \}$, which is variable in position. Schrauf's G Γ g γ are accepted as $o \{ 012 \}$. Schrauf's L Λ l λ , giving $\{ 343 \}$ on the new lattice, probably

² Derived and written in the convenient manner given by Barker (1930, p. 32).

correspond to our $t\{454\}$. Schrauf's II p , giving $\{\overline{17}.3.3\}$ or $\{511\}$ in twin position, are in either case improbable.

Thus Schrauf's formidable list of thirty-nine forms becomes reduced to ten, to which four new ones are added. The author would hesitate to propose such drastic revision of the work of one of the most skillful of the early observers, were it not for the fact that Schrauf evidently failed to make the critical cleavage test on his twinned crystals, and was unable to obtain the optical effects which would have shown that his edifice of twin laws was partly unreal.

TABLE 4. ROSELITE. CORRELATION OF FORMS

Schrauf to Peacock: 0I4/300/030
 Dana to Peacock: $\overline{1}04/0\overline{3}0/300$
 Goldschmidt to Peacock: 40I/060/003

Schrauf 1874	Dana 1892	Goldschmidt 1897, 1922	Peacock 1936
$C\{001\}$	$c\{001\}$	$C\{100\}$	$a\{100\}$
$(Bb)\{010\}$	$a\{100\}$	—	—
$Aa\{100\}$	$b\{010\}$	$A\{010\}$	$b\{010\}$
$(n)\{120\}$	$N\{2\overline{1}0\}$	—	—
$m\{110\}$	$M\{1\overline{1}0\}$	$?m\{012\}$	$\left\{ \begin{array}{l} \overline{1}33 \\ 133 \end{array} \right.$
$M\{1\overline{1}0\}$	$m\{110\}$	$?M\{0\overline{1}2\}$	—
$(N)\{1\overline{2}0\}$	$n\{210\}$	—	—
$(k)\{011\}$	—	—	—
$(K)\{0\overline{1}1\}$	—	—	—
$d\{041\}$	$d\{401\}$	$d\{104\}$	$\left\{ \begin{array}{l} 001 \\ 20\overline{3}=00\overline{1} \text{ twin} \end{array} \right.$
$\Delta\{0\overline{4}1\}$	$\Delta\{401\}$	$\Delta\{104\}$	—
$\eta\{203\}$	$\eta\{0\overline{2}3\}$	$\eta\{310\}$	$\left\{ \begin{array}{l} 210 \\ 2\overline{1}0 \end{array} \right.$
$e\{203\}$	$e\{023\}$	$e\{3\overline{1}0\}$	—
$(x)\{101\}$	$\chi\{0\overline{1}1\}$	—	—
$(h)\{101\}$	$h\{011\}$	—	—
$\phi\{403\}$	$\phi\{0\overline{4}3\}$	$\phi\{320\}$	$\left\{ \begin{array}{l} 110 \\ 1\overline{1}0 \end{array} \right.$
$f\{403\}$	$f\{043\}$	$f\{320\}$	—
$v\{201\}$	$v\{0\overline{2}1\}$	$v\{110\}$	$\left\{ \begin{array}{l} 230 \\ 2\overline{3}0 \end{array} \right.$
$i\{201\}$	$i\{021\}$	$i\{1\overline{1}0\}$	—
$\xi\{803\}$	$\xi\{0\overline{8}3\}$	$\xi\{340\}$	$\left\{ \begin{array}{l} 120 \\ 1\overline{2}0 \end{array} \right.$
$\zeta\{803\}$	$z\{083\}$	$z\{3\overline{4}0\}$	—

TABLE 4. (Continued)

Schrauf 1874	Dana 1892	Goldschmidt 1897, 1922	Peacock 1936
$S\{111\}$	$S\{\bar{1}\bar{1}1\}$	$S\{212\}$	$p\left\{\begin{array}{l} 111 \\ 53\bar{3}=\bar{1}\bar{1}\bar{1} \text{ twin} \\ 5\bar{3}3=\bar{1}\bar{1}\bar{1} \text{ twin} \\ 1\bar{1}\bar{1} \end{array}\right.$
$\Sigma\{1\bar{1}1\}$	$\Sigma\{\bar{1}\bar{1}1\}$	$\Sigma\{2\bar{1}2\}$	
$s\{\bar{1}\bar{1}1\}$	$s\{\bar{1}\bar{1}1\}$	$s\{2\bar{1}2\}$	
$\sigma\{111\}$	$\sigma\{111\}$	$\sigma\{2\bar{1}2\}$	
$O\{221\}$	$O\{221\}$	—	$q\left\{\begin{array}{l} 13\bar{3}=\bar{1}\bar{1}1 \text{ twin} \\ 11\bar{1} \\ 1\bar{1}\bar{1} \\ 1\bar{3}3=\bar{1}\bar{1}\bar{1} \text{ twin} \end{array}\right.$
$\Omega\{221\}$	$\Omega\{221\}$	$\Omega\{\bar{1}\bar{1}2\}$	
$o\{221\}$	$o\{221\}$	$o\{\bar{1}\bar{1}2\}$	
$\omega\{221\}$	$\omega\{221\}$	—	
$G\{241\}$	$G\{421\}$	$?G\{114\}$	$o\left\{\begin{array}{l} 012 \\ 43\bar{6}=01\bar{2} \text{ twin} \\ 4\bar{3}6=0\bar{1}2 \text{ twin} \\ 0\bar{1}2 \end{array}\right.$
$\Gamma\{2\bar{4}1\}$	$\Gamma\{\bar{4}21\}$	—	
$g\{241\}$	$g\{421\}$	$g\{\bar{1}14\}$	
$\gamma\{241\}$	$\gamma\{421\}$	—	
$L\{433\}$	$L\{343\}$	$L\{323\}$	— $\left\{\begin{array}{l} 343 \\ 54\bar{3}=\bar{3}4\bar{3} \text{ twin} \\ 54\bar{3}=\bar{3}4\bar{3} \text{ twin} \\ 343 \end{array}\right.$
$\Delta\{433\}$	$\Delta\{343\}$	$\Delta\{323\}$	
$l\{433\}$	$l\{343\}$	—	
$\lambda\{433\}$	$\lambda\{343\}$	$\lambda\{323\}$	
$\Pi\{1\bar{1}4\}$	—	$\Pi\{8\bar{1}2\}$	— $\left\{\begin{array}{l} 17.3.\bar{3}=\bar{5}\bar{1}\bar{1} \text{ twin} \\ 17.\bar{3}.3=\bar{5}\bar{1}\bar{1} \text{ twin} \end{array}\right.$
$p\{\bar{1}\bar{1}4\}$	—	$p\{812\}$	
—	—	—	$k\{350\}$
—	—	—	$r\{238\}$
—	—	—	$s\{122\}$
—	—	—	$t\{454\}$

OPTICS

The first optical tests, made on small measured crystals of the light rose kind (H.M.M. 93835), tended to confirm Schrauf's conclusion, that the principal optical directions practically coincide with his crystallographic axes, that is with the edges of the pseudo-orthorhombic cell *EBFD* (Fig. 7). Such crystals, single or twinned, lying on any face in the zone [001], extinguish sensibly as a whole parallel to [001]; with [001] in the axis of the microscope they extinguish parallel to the trace of the cleavage {010}. In thin cleavage plates, however, split from measured twins on (100), the trace of the twin plane can be seen, and slightly oblique symmetrical extinction can sometimes be detected, a principal optical direction being inclined to [001] at 0° to 1° in the obtuse axial angle β . Such plates show lively pleochroism in shades of rose-red and

fairly strong double refraction. Further study of small crystals, cleavage plates and grains gave the following optical data, the absorption colours being those shown by grains of the order of 0.01 mm. in thickness.³

		<i>n</i> (Na)	
X (pale rose) : [001]=+ 0° to 1°	1.694	} ±0.003	Positive
Y (paler rose) =[010]	1.704		2 <i>V</i> =75°
Z (palest rose) : [001]=+90° to 91°	1.719		<i>r</i> < <i>v</i>

Cleavage plates from the dark rose crystals (H.M.M. 93836), present an appearance which is surprisingly different from that of the light rose material. The dark rose crystals prove to be strongly zoned in shells whose outlines conform to those of the principal forms {111}, { $\bar{1}11$ }, and {210}. Cleavage plates from measured twins on (100) show symmetrical extinction about the trace of the twin plane, a principal optical direction being inclined to [001] at 12° to 20° in the obtuse axial angle β , the angle of extinction increasing in the outer zones. The multiple and somewhat variable reflections given by the bounding planes of many of the crystals may be referred to slight distortion due to an increasing misfit between successive zones that differ in optics and therefore in chemical composition and crystallographic form. The full optical data for the dark rose crystals are as follows:

		<i>n</i> (Na)	
X (deep rose)=[010]	1.725	} ±0.003	Positive
Y (pale rose) : [001]=+12° to 20°	1.728		2 <i>V</i> =60°
Z (paler rose) : [001]=-78° to 70°	1.735		<i>r</i> < <i>v</i>

The two kinds of roselite have the same pleochroic formula, the same optical sign, and similar optic axial angle and dispersion; they differ, however, in having noticeably different indices of refraction and entirely different optical orientations. The darker colour and stronger refraction of the dark rose crystals are in keeping with Schrauf's determinations of composition and specific gravity, which showed that the dark crystals from Rappold are richer in cobalt and higher in specific gravity than the light red crystals from the Daniel mine. Possibly we are dealing with distinguishable varieties, and, in the case of the dark crystals, with an isomorphous series; but with insufficient material for adequate analyses this question could not be pursued.

COMPOSITION

Schrauf's analyses on minute quantities led him to the formula $\text{Ca}_7\text{Mg}_2\text{Co}_3\text{As}_8\text{O}_{52} \cdot 10\text{H}_2\text{O}$ for light rose crystals from Daniel, and

³ Mr. Berman kindly made independent optical measurements on the new roselite material, obtaining results which agree with those of the author within the expected limits of error.

$\text{Ca}_6\text{Mg}_2\text{Co}_4\text{As}_8\text{O}_{52} \cdot 10\text{H}_2\text{O}$ for dark rose crystals from Rappold. On larger quantities Winker (1877) derived the simpler formula $(\text{Ca}, \text{Co}, \text{Mg})_3\text{As}_2\text{O}_8 \cdot 2\text{H}_2\text{O}$ for roselite. Until further chemical data are available it is proper to follow Dana (1892) and accept Winkler's formula, which is comparable to that of several other natural arsenates and phosphates.

RELATION TO BRANDTITE

When the foregoing work was completed, the description of brandtite— $\text{Ca}_2\text{MnAs}_2\text{O}_8 \cdot 2\text{H}_2\text{O}$, was examined to see how the new setting of roselite would affect the accepted homeomorphism of the two species. Following Nordenskiöld (in Lindström, 1891), Dana (1892) described brandtite as triclinic, similar in form to roselite, but without geometrical elements. Turning to the later work it was a pleasure to find that the crystallography of brandtite had been revised by Aminoff (1919), who found, as we have in the case of roselite, that brandtite is monoclinic, holohedral, with cleavage $\{010\}$ and common twin plane (100). The following comparative data show how closely the two species agree in form:

Brandtite— $\text{Ca}_2\text{MnAs}_2\text{O}_8 \cdot 2\text{H}_2\text{O}$	Roselite— $(\text{Ca}, \text{Co}, \text{Mg})_3\text{As}_2\text{O}_8 \cdot 2\text{H}_2\text{O}$							
$a:b:c=0.8720:1:0.4475$;	$a:b:c=0.8780:1:0.4398$;							
$\beta=99^\circ 36\frac{1}{2}'$ (Aminoff, 1919)	$\beta=100^\circ 53'$ (Peacock, 1936)							
Forms in common:	$\{010\}$	$\{100\}$	$\{120\}$	$\{230\}$	$\{110\}$	$\{210\}$	$\{111\}$	$\{\bar{1}\bar{1}\bar{1}\}$
Brandtite.....	A	C	ζ	v	ϕ	η	S	R
Roselite.....	b	a	j	l	m	n	p	q
Calculated angles:								
	ϕ	ρ			ϕ		ρ	
$\phi(110)$	$49^\circ 19'$	$90^\circ 00'$		$m(110)$	$49^\circ 14'$		$90^\circ 00'$	
$S(111)$	$57^\circ 01\frac{1}{2}'$	$39^\circ 25\frac{1}{2}'$		$p(111)$	$57^\circ 57'$		$39^\circ 39'$	

Both roselite and brandtite are stout columnar after $[001]$, and both have $\{010\}$, $\{111\}$, and $\{210\}$ as the principal forms. It is interesting to note that Aminoff chose what are undoubtedly the proper axes for brandtite even though the base $\{001\}$ is not known, and that he adopted a plane giving similar parameters to those of roselite, after considering, as we did, the possibility of taking $\{212\}$ as the unit form. Finally, the optical orientation of brandtite is similar to that of light rose roselite. The homeomorphism of the two species is complete, and there can be little doubt that their ultimate structures must be very similar.

CONCLUSION

The foregoing morphological study has shown that the lattice of roselite with the highest pseudo-symmetry is not the proper crystal lattice of the species, but a multiple lattice; and that the plane of common twinning is a plane of pseudo-symmetry in the multiple lattice but

not in the crystal lattice. The same is true in many other species, and in all such cases the Rule of Highest Pseudo-Symmetry leads to improper crystallographic elements. This was clearly recognized by Friedel (1904), who exposed many crystallographic crudities resulting from the ill-considered application of the Rule of Highest Pseudo-Symmetry.⁴ Prior to Friedel, the French School regarded all twinning elements as elements of symmetry or pseudo-symmetry of the crystal lattice; this, in effect, made the Rule of Highest Pseudo-Symmetry a theoretical necessity and served to justify the many clearly unnatural settings demanded by this rule. Friedel found the true solution in admitting that elements of twinning are in many cases elements of symmetry or pseudo-symmetry in a multiple lattice of the crystal lattice. Formally, Friedel expressed this significant development of the theory of twinning by adding "twinning by reticular merohedry" and "twinning by reticular pseudo-merohedry" to Mallard's "twinning by merohedry" and "twinning by pseudo-merohedry."

Friedel approached the discussion of twins from the point of view of the Law of Bravais, namely by finding the lattice which gives the best correspondence between the reticular densities of the known planes and their observed relative importance. The proper crystal lattice having been determined in a given case, it is at once evident whether the elements of twinning are elements of symmetry or pseudo-symmetry of the crystal lattice or whether they are elements of symmetry or pseudo-symmetry in a multiple lattice of the crystal lattice; or, in other words, whether the lattice with the highest pseudo-symmetry is the crystal lattice or a multiple lattice of the crystal lattice.

While this method leads, at least in the majority of cases, to the true solution, it is well known that the Law of Bravais is only a first approximation and that, in many actual cases, there is lack of detailed agreement between relative importance of crystal planes and their reticular densities on any lattice that may be chosen. Indeed, there are cases in which the Law of Bravais does not give an unequivocal solution, and there are others in which the law leads to a result which is different from that indicated both by the principle of simplest indices and by the röntgenographically determined translation lattice. Such cases cause one to question the value of the Law of Bravais as a basic guiding principle in determining a crystal lattice.

The writer's experience leads him to the conviction that the proper crystal lattice can be determined from morphological data by simple inspection of the indices of the known forms, without subscribing to the

⁴ I am obliged to Professor J. D. H. Donnay for drawing my attention to Friedel's valuable work on twinning.

belief in a strict relation between reticular density and form importance. And thus he finds himself in a position similar to that adopted by Ungemach. The details of the procedure whereby the lattice is determined from the indices cannot be enumerated and explained here. In simple cases, like the present one, the widely used principle of simplest indices leads directly to the proper solution.

Pseudo-symmetry remains a crystallographic fact of fundamental significance, and the search for the lattice with the highest pseudo-symmetry is part of every serious morphological study. But to adopt this lattice as the crystal lattice in every case, at the cost of complicating the indices and forcing a pseudo-symmetry which is not expressed in the form development, is contrary to good crystallographic principles and practice.

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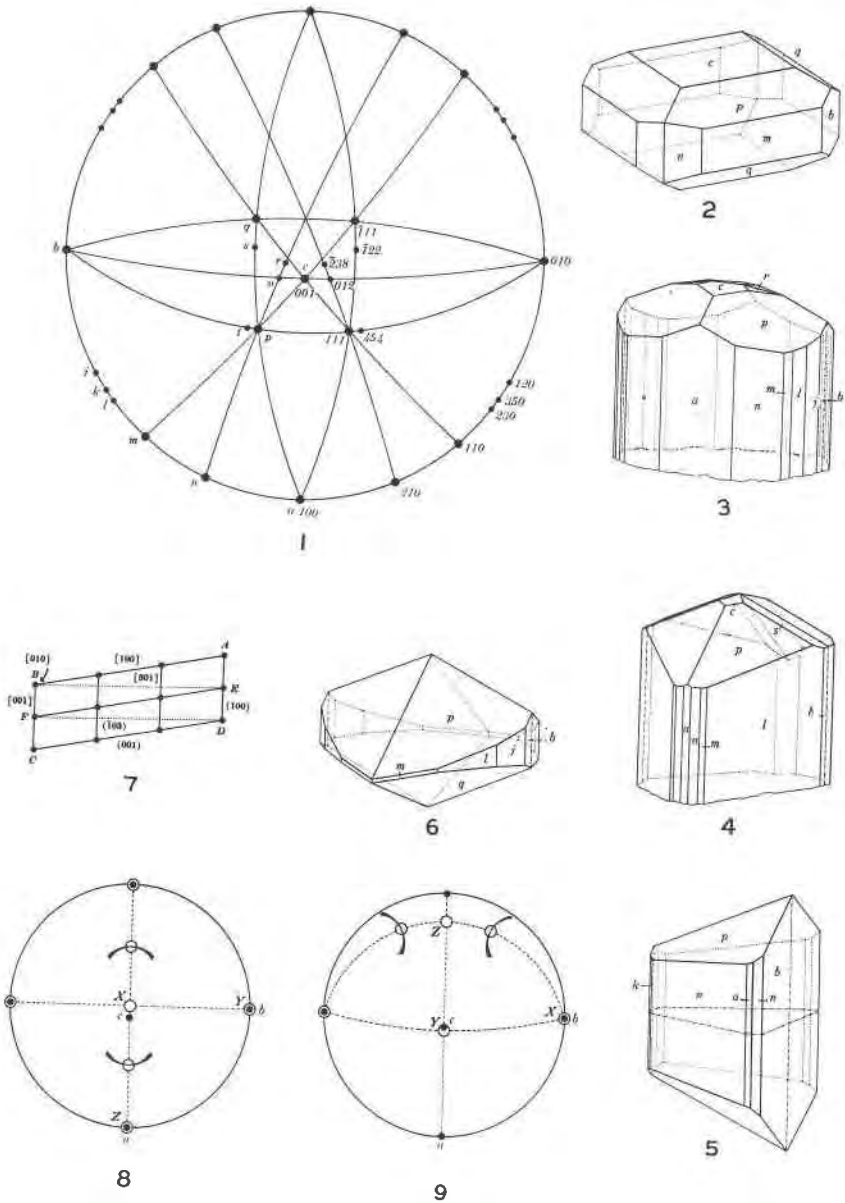


FIG. 1. Roselite from Schneeberg, Saxony; stereographic projection of the accepted forms.

FIG. 2. Single crystal, thick tabular after the base.

FIGS. 3, 4, 6. Contact twins on $a(100)$.

FIG. 5 Fourling of "Roc tourné" type.

FIG. 7. Morphological lattice projected on (010) , showing six cells of the monoclinic crystal lattice and one cell of the pseudo-orthorhombic twin lattice.

FIG. 8. Optical orientation of the light red crystals.

FIG. 9. Optical orientation of the dark red crystals.