RE-ORIENTATION OF RÖMERITE

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Römerite—$Fe_2'''Fe''(SO_4)_4 \cdot 14H_2O$, from near Goslar in the Harz, was named by Grailich (1858). The first adequate crystallographic work on the species was that of Blaas (1884) who studied crystals from Persia and obtained triclinic elements which were adopted with minor corrections by Goldschmidt in the *Index* (1891). Linck (1888) measured crystals of römerite from Chile and computed triclinic elements in a new setting; these are given in corrected form by Dana (1892). Scharizer (1913) took still another position, computing new elements from Linck's measurements; these are reproduced, with a considerable change in the *a*-axis, by Doelter (1927). Finally, Ungemach (1935) adopted Linck's setting in preference to that of Blaas, and calculated new elements considerably different from those of Linck, from careful measurements on crystals with many new forms from Tierra Amarilla in Chile. Römerite thus presents a situation which is common among triclinic species, namely a multiplicity of published crystallographic orientations representing only a few of the scores of settings which will satisfy the usual loosely defined requirements of an acceptable triclinic orientation.

In preparing a definitive crystallographic presentation the choice of setting requires first consideration. If there is a unique setting that expresses generally accepted morphological and structural requirements and can easily be reached by different workers, such a setting has great advantages over an arbitrary orientation. The normal triclinic setting of Peacock (1937) meets these requirements. It is defined as the unique setting in which the geometrical elements correspond to the cell given by the three shortest non-coplanar identity periods in the structural lattice, in the one orientation in which the axis of the main zone is *c*[001], the axial angles α and β are both obtuse, and the axis *b*[010] is longer than the axis *a*[100]. From this definition it follows that the axial planes are the three planes with the greatest spacings in the structural lattice; consequently, the reciprocal axial periods are also the three shortest periods in the reciprocal structural lattice. The condition that α and β are both obtuse results from the conventional attitude of the base, which slopes to the front-right ($\phi_{001} = 0°$–$90°$); while the condition that *b*[010] is greater than *a*[100] causes the projected reciprocal lattice period p_0' to be greater than the projected period q_0'. A common, but not infallible, consequence of the normal setting is that [001] is the shortest direct lattice period, while (010) is the plane with the greatest spacing and therefore the most probable cleavage.

Peacock (1937) and Richmond (1937) have shown how the normal

setting can be found from the external geometry of triclinic crystals, the correctness in both cases being proved by subsequent, independent determinations of the structural lattices. In the present case a confirmatory röntgenographic determination is unnecessary, since the gnomonic projection of the forms on the plane normal to the axis of the main zone presents the perfectly ideal aspect of the normal setting. In the papers mentioned the method of recomputing triclinic elements to a new setting is not explained; and since this process is not concisely given in the accessible texts an outline of the method may be useful.

The forms of römerite in Linck's position, according to Ungemach (1935, p. 161), are shown in stereographic projection in figure 1. One observes the weakness of the vertical zone [001], which has only three forms; the steepness of the parametral plane (111), yielding a relatively long vertical axis; and the marked eccentricity of the pole of the base (001), indicating axes of considerable obliquity. These features are all at variance with the principles of the normal setting.

Linck's zone [(001)(010]=[100], with twelve forms, is clearly the main zone; this is supported by Ungemach's words: "La zone $p\ g^1$ est toujours richement développée." Allowing for the viewpoint adopted in Ungemach's figures 18 and 19, the axis [100] also appears to be the axis of morphological elongation. Swinging the poles in our figure 1 forward about the normal to (010) until (001) falls into the primitive circle, projecting each stereographic point into its gnomonic position, and turning the combined stereographic-gnomonic projection about the vertical axis into the one position in which the requirements of the normal setting are satisfied, we obtain the relations in figure 2. In this figure the small points are the stereographic points in the new position; the larger filled points are the gnomonic points of the terminal planes; the radial lines drawn from (001) to ($hk1$) are normals to the vertical planes ($hk0$).

Since the gnomonic terminal points fall without exception at the nodes of a plane lattice, this lattice is unquestionably the first layer of the reciprocal structural lattice. The three shortest periods in this reciprocal lattice are: $p_0' = (001)-(101) = (000)-(100)$; $q_0' = (001)-(011) = (000)-(010)$; $r_0' = (000)-(001)$. The lengths p_0', q_0', are measured directly on the gnomonic projection; r_0', the distance from (001) to the center of the sphere of projection, is obtained by a simple construction. The reciprocal axial angles $\lambda = (010):(001)$, $\mu = (001):(100)$, $\nu = (100):(010)$, are most easily measured in the stereographic projection. Thus we obtain graphical values for the elements of the new reciprocal lattice which are useful in checking subsequent calculations.

In the normal setting Linck's axial planes and parametral plane receive new symbols, as follows:

Linck	Wolfe
(100)	= (00$\bar{1}$)
(010)	= (1$\bar{1}$0)
(001)	= (0$\bar{1}$0)
(111)	= (12$\bar{1}$)

This equivalence gives the transformation formula, Linck to Wolfe: 010/01$\bar{1}$/$\bar{1}$00, whereby all Ungemach's face symbols are rapidly transformed to the new setting.

The transformation formula has another property which is invaluable in the present connection; it gives directly the symbols [*uvw*] of the new axes in the old lattice, which we require for computing the new lattice elements, a', b', c'; α', β', γ', from the old lattice elements, a, b, c; α, β, γ. We can write at once:

Wolfe		Linck		
a'[100]	=	[010]	=	b
b'[010]	=	[0$\bar{1}\bar{1}$]	=	—
c'[001]	=	[$\bar{1}$00]	=	$-a$
α'=[010]:[001]	=	[0$\bar{1}\bar{1}$]:[$\bar{1}$00]	=	—
β'=[001]:[100]	=	[$\bar{1}$00]:[010]	=	180^0-γ
γ'=[100]:[010]	=	[010]:[0$\bar{1}\bar{1}$]	=	—

Only three of the new elements, namely b', α', γ', require to be computed. The length b' we obtain from the general formula: $T^2_{uvw}=a^2u^2+b^2v^2+c^2w^2+2bcvw\cos\alpha+2cawu\cos\beta+2abuv\cos\gamma$, where T_{uvw} is the translation distance (identity period) in the old lattice row [*uvw*]. The angles α', γ', are obtained by the general expression: $\cos\tau=[a^2u_1u_2+b^2v_1v_2+c^2w_1w_2+bc(v_1w_2+w_1v_2)\cos\alpha+ca(w_1u_2+u_1w_2)\cos\beta+ab(u_1v_2+v_1u_2)\cos\gamma]/T_{u_1v_1w_1}\cdot T_{u_2v_2w_2}$, in which τ is the angle between the rows $[u_1v_1w_1]$ and $[u_2v_2w_2]$ in the old lattice. In this case, as in most special cases, many terms vanish in the general equations. In computing lattice angles it is necessary to write the symbols of the lattice rows in proper cyclic order to ensure that the value of the cosine of the angle sought has the proper sign.

The correctness of the foregoing calculations can be verified by calculating the volumes of the elementary cells from both sets of elements from the formula:

$$V = abc\sqrt{(1 + 2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma)}.$$

The volumes are bound to be integrally related; in the present case they are identical, since both cells are unit cells of the same lattice; the value obtained from both sets of elements is $V=2.3035$.

Thus from Ungemach's elements for römerite in Linck's setting:

$a:b:c=0.99035:1:2.6460$; $\alpha=116°37'$, $\beta=95°06'$, $\gamma=79°30'$

we obtain the normal elements:

$a':b':c' = 0.4214:1:0.4174$; $\alpha' = 91°17'$, $\beta' = 100°30'$, $\gamma' = 85°31'$

In conclusion we give a presentation of the morphological crystallography of römerite which follows the form used by Palache in Peacock (1937). The addition of Dana's form letters, which are often used alone in describing crystal forms, permits ready correlation of the old and new notations.

RÖMERITE[1]—$Fe_2'''Fe''(SO_4)_4 \cdot 14H_2O$

Triclinic; pinacoidal—$\bar{1}$

$a:b:c = 0.4214:1:0.4174$; $\alpha = 91°17'$, $\beta = 100°30'$, $\gamma = 85°31'$[2]
$p_0:q_0:r_0 = 0.9931:0.4116:1$; $\lambda = 89°31\frac{1}{2}'$, $\mu = 79°34'$, $\nu = 94°19\frac{1}{2}'$
$p_0' = 1.0101$, $q_0' = 0.4186$; $x_0' = 0.1853$, $y_0' = 0.0084$

Forms[3]		ϕ	ρ	A	B	C	Dana
c	001	87°24½′	10°30′	79°34′	89°31½′	0°00′	a
b	010	0 00	90 00	94 19½	0 00	89 31½	c
a	100	94 19½	90 00	0 00	94 19½	79 34	q
i	140	32 13	90 00	62 06½	32 13	84 01½	—
j	130	40 29	90 00	53 50	40 29	82 51	l
k	120	52 55	90 00	41 24	52 55	81 21½	s
m	110	71 13	90 00	23 06½	71 13	79 55	n
N	$2\bar{1}0$	105 49½	90 00	11 30	105 49½	80 02½	—
M	$1\bar{1}0$	116 10	90 00	21 50½	116 10	80 47½	b
L	$2\bar{3}0$	124 57½	90 00	30 38	124 57½	81 41½	—
K	$1\bar{2}0$	132 12½	90 00	37 53	132 12½	82 34	e
J	$1\bar{3}0$	142 54½	90 00	48 35	142 54½	84 04½	—
I	$1\bar{4}0$	150 05½	90 00	55 46	150 05½	85 12	—
w	011	23 26½	24 57½	82 03½	67 13½	22 18½	—
x	021	12 21	40 53	84 45½	50 15½	39 16½	—
W	$0\bar{1}1$	155 42½	24 14	78 40	111 58	22 26½	x
X	$0\bar{2}1$	167 24½	40 20½	79 08½	129 11	39 39½	—
Y	$0\bar{3}1$	171 33½	51 35½	80 02	140 49	51 17	—
d	101	93 15	50 03½	39 57	99 29½	39 37	—
D	$\bar{1}01$	−84 07½	39 34	129 33	86 16	49 59	—
p	111	73 36	51 11	43 13	77 17½	41 02½	—
r	$\bar{1}11$	−58 31½	43 56½	128 08	68 45½	52 54	m
t	$\bar{1}\bar{1}1$	−112 07½	41 35	126 33½	104 28½	51 35	—
q	121	57 10	54 50	49 21	63 41½	45 58	—
s	$\bar{1}21$	−41 43½	51 00	124 01	54 32½	58 02½	—
u	$\bar{1}\bar{2}1$	−132 20	43 06	120 37½	120 11	56 27½	—

Habit: Cuboidal, with prominent development of the axial zones; thick tabular {010} In crystal aggregates; granular.

Cleavage: {010} perfect; also {001}, less good.

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[1] Grailich (*Ber. Akad. Wien*, **28,** 272, 1858).

[2] Ungemach (*Bull. Soc. franç. Min.*, **58,** 162, 1935), on crystals from Chile, transformed to the normal setting. Ungemach retained the setting of Linck (*Zeits. Krist.*, **15,** 23, 1888) which was also accepted by Dana (*System*, 1892). Goldschmidt (*Winkeltabellen*, 1897; *Atlas*, **7,** 1922) took another position. The adopted axial directions agree with those of Blaas (*Ber. Akad. Wien*, **88** (1), 1121, 1884), as corrected by Goldschmidt (*Index*, **3,** 45, 1891), if allowance is made for his poor measurements.

Transformations: Blaas to normal position. 100/020/001; Linck to normal position 010/0$\bar{1}$1/$\bar{1}$00; Goldschmidt to normal position: 0$\bar{1}$0/$\bar{1}$00/00$\bar{1}$.

[3] Ungemach (1935), relettered; the following forms of Linck (1888) are rejected as erroneous: m\{320\}, y\{508\}, t\{0.$\bar{5}$.18\} (Linck's notation).

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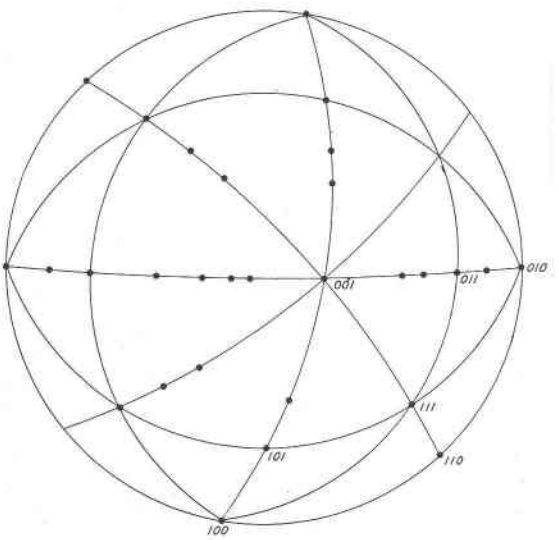

FIG. 1. Römerite: stereographic projection of the accepted forms, after Ungemach (1935). The position is that of Linck (1888), adopted by Dana (1892).

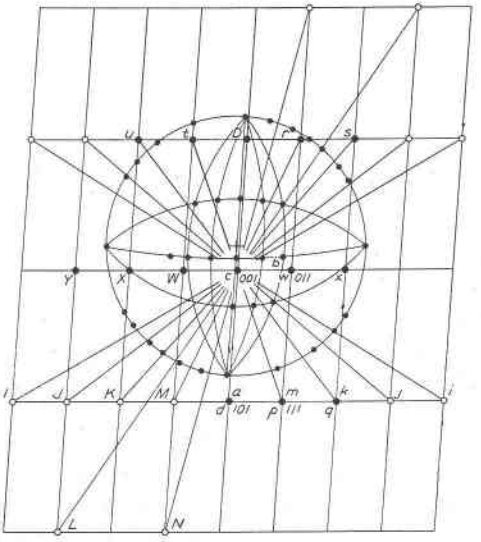

FIG. 2. Römerite: stereographic-gnomonic projection of the accepted forms in normal position.

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