RE-ORIENTATION OF RÖMERITE


Römerite—$\text{Fe}_2''\text{Fe}''(\text{SO}_4)_4 \cdot 14\text{H}_2\text{O}$, from near Goslar in the Harz, was named by Grallich (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 $\alpha$ and $\beta$ 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 $\alpha$ and $\beta$ are both obtuse results from the conventional attitude of the base, which slopes to the front-right ($\phi_{001} = 0^\circ$–$90^\circ$); 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

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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' 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 (hk0) 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:
This equivalence gives the transformation formula, Linck to Wolfe: 010/011/100, 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, $a', b', c'; \alpha', \beta', \gamma'$, from the old lattice elements, $a, b, c; \alpha, \beta, \gamma$. We can write at once:

<table>
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<th>Wolfe</th>
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<tr>
<td>[100]</td>
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<td>[010]</td>
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Only three of the new elements, namely $b', \alpha', \gamma'$, require to be computed. The length $b'$ we obtain from the general formula: $T_{uvw}^2 = a^2u^2 + b^2v^2 + c^2w^2 + 2bcuw \cos \alpha + 2cawu \cos \beta + 2abuw \cos \gamma$, where $T_{uvw}$ is the translation distance (identity period) in the old lattice row [uvw]. The angles $\alpha', \gamma'$, are obtained by the general expression: $\cos \tau = \frac{a^2u_1u_2 + b^2v_1v_2 + c^2w_1w_2 + bc(v_1u_2 + w_1v_2)}{T_{uvw}} \cos \alpha + \frac{ca(u_1u_2 + v_1w_2)}{T_{uvw}} \cos \beta + \frac{ab(v_1u_2 + w_1v_2)}{T_{uvw}} \cos \gamma$, in which $\tau$ is the angle between the rows [uvw] and [uvw] 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 romerite in Linck's setting:

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

we obtain the normal elements:
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\textsuperscript{1}—Fe\textsuperscript{2+}/Fe\textsuperscript{3+}(SO\textsubscript{4})\textsubscript{4}·14H\textsubscript{2}O

Triclinic; pinacoidal—\textit{I}

\[ a:b:c = 0.4214:1:0.4174; \quad \alpha' = 91^\circ 17', \beta' = 100^\circ 30', \gamma' = 85^\circ 31' \]

<table>
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<th>(B)</th>
<th>(C)</th>
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</tr>
</tbody>
</table>
Habit: Cuboidal, with prominent development of the axial zones; thick tabular \{010\} in crystal aggregates; granular.
Cleavage: \{010\} perfect; also \{001\}, less good.

1 Graillich (Ber. Akad. Wien, 28, 272, 1858).
2 Ungemach (Bull. Soc. franc. 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 010/011/100; Goldschmidt to normal position: 010/100/001.
3 Ungemach (1935), relettered; the following forms of Linck (1888) are rejected as erroneous: m\{320\}, y\{508\}, t\{0.5.18\} (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.

REFERENCES

GOLDSCHMIDT, V. (1891): Index der Krystallformen, 3—Berlin.