

thorium content of 83.6 weight%. The compound formed at 700° C. and below could be isolated only by mechanical separation of the dendritic crystals. Analyses of these samples found 78 weight% thorium. Small amounts of the magnesium-rich matrix could easily have adhered to the samples of the low-temperature form. Accurate density determinations could not be made because of the small sample size. The analytical results indicated that the compounds were very close to ThMg₂.

Crystals of both compounds were examined by X-ray diffraction with a Weissenberg camera. The high-temperature form was found to belong to the space group *Fd3m* and have a lattice constant of 8.570 Å. The compound has the Cu₂Mg, *C15* structure and is therefore a Laves phase. The analysed composition of the phase and the qualitative agreement between calculated and observed intensities leave no doubt as to the structure. There are no parameters involved in the location of the atoms.

The low-temperature form was found to belong to the space group *C6/mmc* and to have the Ni₂Mg, *C36* structure. The lattice constants are: $a_0 = 6.086$ Å, $c_0 = 19.64$ Å. The axial ratio c/a is 3.23. This structure involves several parameters. The parameters reported in *Strukturbericht* for Ni₂Mg were used for a trial structure. The calculated intensities agreed very well with the observed intensities

for Weissenberg patterns through the fourth layer and for 00*l* precession patterns. No attempt was made to refine the atomic parameters because the magnesium atoms could not be located precisely, owing to their small contribution to the intensities. The calculation of the position of the thorium atoms must be quite accurate in order to have given the excellent qualitative agreement of the calculated and observed intensities.

These compounds seem to belong to the family of Laves phases and are additional examples of the formation of one type at high temperature and another at a lower temperature. The cubic, high-temperature form does not transform readily into the hexagonal modification. Samples were observed to contain crystals of both types even after heating at 700° C. for 48 hr.

The radius ratio for magnesium to thorium radii is 0.889. Closest bond distances in the two structures are:

	Th-Th	Th-Mg	Mg-Mg
Cubic	3.711 Å	3.553 Å	3.029 Å
Hexagonal	3.69	3.53	3.04

The bond distances for the hexagonal compound are not as accurate as those for the cubic compound. The distances are very nearly the same in both forms, as would be expected from the structural similarity.

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A graphical aid for the rapid evaluation of absorption corrections by Albrecht's method.

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The labour of estimating absorption corrections by Albrecht's (1939) method can be considerably reduced with the aid of the following simple procedure.

An outline of the cross-section of the crystal is drawn on tracing paper to a scale such that dimensions of length x correspond to true lengths, x' , by the relation

$$x = \mu x',$$

where μ is the linear absorption coefficient of the crystal, and m is a constant (see below). This is pinned down permanently in the correct orientation over the corresponding reciprocal lattice (see the bold outline *EFGH* in Fig. 1). Over this again are placed two transparent sheets marked in their overlapping parts with uniformly spaced parallel lines. They are pinned to the board at O , the origin of the reciprocal net, and are rotated for each reflexion so that one set of rulings, I , is parallel to the incident rays; the other, D , to the diffracted rays. This is greatly facilitated if both sheets carry a Bernal circle to match the underlying reciprocal lattice: both circles are arranged to intersect at S , the reciprocal-lattice point.* The absorption suffered by a reflexion could be

estimated by listing $(l_1 + l_2)$ (Fig. 1) for as many (N) points of intersection of the ray rulings as are necessary, and then subsequently evaluating

$$A = N^{-1} \sum \exp [-(l_1 + l_2)/m].$$

We have, however, found it especially convenient to use a transparent rule, *RR'* (Fig. 1), graduated to read $\exp[-x/m]$, where x is in cm. This is laid along the incident ray with its origin at the point of entry into the crystal. Using a pair of dividers, one may find the point Q on the scale corresponding to $(l_1 + l_2)$ from the origin and so read off the attenuation directly. This is quickly repeated for $P_1 - P_7$, and, after a shift of the ruler, for P_8 etc. The factors are accumulated in a desk adder. The graduations of *RR'* are most conveniently copied from the *C*(10:1) or *D*(100:1) scales of any 10 in. or 25 cm. slide rule. The corresponding values of m are 11.03 (10 in.) and 10.86 (25 cm.) for the *C* scale, and half these for the *D* scale. It is advisable to mark the ruler with the appropriate factor.

Heavily absorbing crystals are represented by large sections and so have many points of intersection of the ray rulings. If the rulings are coloured alternately red and black, one can, by using either red-red (or black-black), red-black, or all the intersections, sample at uniformly spaced points representing either one quarter, one half, or all of the available intersections.

If, for weakly absorbing crystals, the cross-section is fairly regular, the variation of A throughout most of

* Incidentally, when used in this way, these sheets are convenient for the recognition and interpretation of cases of 'Umweganregung', the Renninger (1937) effect. This will occur if another lattice point T also falls on the *D*-circle, and if both reflexions S , T are strong. The simulated reflexion corresponds to a point U on the *I*-circle.

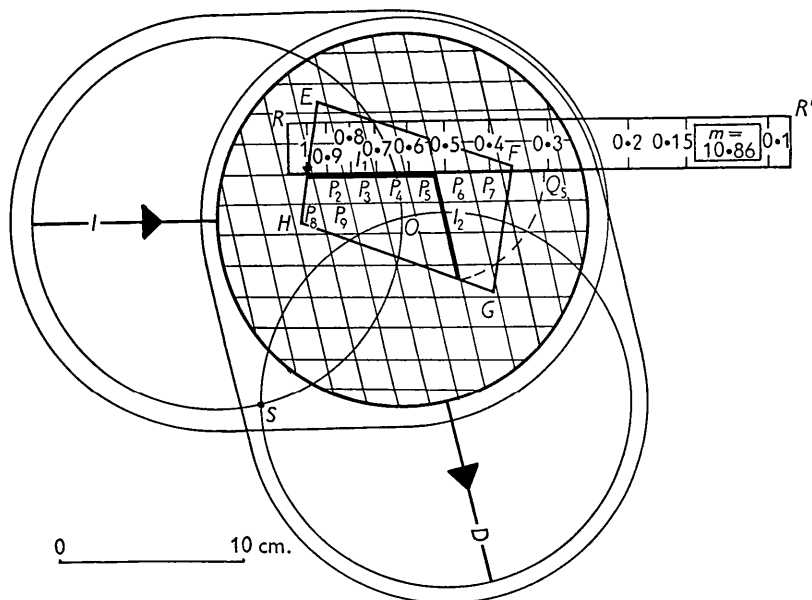


Fig. 1. $EF GH$ represents the enlarged outline of the cross-section of the crystal. I, D are the two sheets of ray rulings, incident and diffracted respectively. The Bernal circles are set to intersect at S , a point of the reciprocal lattice, but for clarity the reciprocal net is not shown. The ray diffracted at P_5 has a total path length of $(l_1 + l_2)$. The exponential ruler is shown as RR' , and the use of the dividers to find the point Q_5 is obvious.

reciprocal space is smooth and slight. Sufficiently accurate values can, therefore, often be obtained by evaluating A at a few reciprocal-lattice points, drawing contours of A , and interpolating at the remaining points.

References

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Orthorhombic rhenium dioxide: a representative of a hypothetical structure type predicted by Pauling & Sturdivant. By ARNE MAGNÉLI, *Institute of Inorganic and Physical Chemistry, University of Stockholm, Stockholm, Sweden*

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By heating ammonium perrhenate at 500°C . *in vacuo* Zachariassen (1951, also private communication) obtained rhenium dioxide, the crystal structure of which was found to be of the monoclinic MoO_2 type. If the reaction is carried out at higher temperatures an orthorhombic modification of rhenium dioxide is obtained. This phase also results when appropriate mixtures of rhenium and rhenium trioxide are heated in a sealed, evacuated silica tube. By prolonged heat-treatment (a few weeks) at about 1050°C . minute, greyish crystals, suitable for single-crystal work, have been obtained.

X-ray studies of the latter phase (by Weissenberg and Guinier photographs) have made possible the determination of the rhenium positions and a discussion of the probable oxygen arrangement. The following structural data are thus obtained:

$$a = 4.810, b = 5.643, c = 4.601 \text{ \AA}.$$

Cell content: 4ReO_2 .

Space group: $Pbcn$ (No. 60 of *International Tables for X-ray Crystallography*, vol. 1, 1952).

$$4 \text{Re in } 4(c), y = 0.110.$$

$$8 \text{O in } 8(d), x = 0.25, y = 0.36, z = 0.125.$$

The structure may be described as built up of ReO_6 octahedra by sharing edges to form staggered strings of the same type as those present in brookite. However, the strings are mutually connected in the same way as the straight strings of rutile, namely, by shared corners.

It is of interest to notice that this atomic arrangement coincides with a hypothetical structure type (called 'A') discussed by Pauling & Sturdivant (1928) in connexion with the determination of the brookite structure. (The paper of these authors presents a photograph of a model of the structure, which is related to the columbite structure type (Sturdivant, 1930).) Assuming regular octahedra, the ideal parameter values of the model would read:

$$y (M) = 0.125;$$

$$x (O) = 0.250, y (O) = 0.375, z (O) = 0.125.$$

The pronounced difference between the axial ratio of