



Fig. 1. $EFGH$ 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

the rhenium dioxide structure ($a:b:c = 1.045:1.226:1$) and that of the ideal model ($a:b:c = 0.944:1.155:1$) is probably related to the short Re-Re distance within the strings (2.61 Å), which suggests the presence of Re-Re bonds. This is likely to force the oxygen atoms of shared edges apart; this will widen the structure in the a and b directions and more so in the former. Similar deformations due to metal-metal interaction in chains of metal-oxygen octahedra have previously been observed in molybdenum dioxide (Magnéli, 1946).

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Unit cell and space group of some amino acids. By R. SRINIVASAN, *Department of Physics, University of Madras, Madras 25, India*

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As part of the work in this laboratory on the structure of proteins, the structure analysis of some crystalline amino acid derivatives has been undertaken. Preliminary results are reported here for L-tyrosine HCl, L-tyrosine HBr, L-cystine HCl, L-cystine HBr and L-lysine monohydrochloride dihydrate. The first two compounds are isomorphous, and their structures have been worked out by the author using the difference-Patterson technique (Kartha & Ramachandran, 1955) and are now in the final stages of refinement. Detailed examination of the lysine derivative is in progress but the work on the cystine compounds has been discontinued as they are being investigated elsewhere (Steinrauf & Jensen, 1956).

The X-ray data were collected from rotation and Weissenberg photographs, using Cu $K\alpha$ radiation, and morphological investigations were carried out where possible. The densities of the crystals were determined by flotation in bromoform and benzene. The results are summarized in Table 1. The accuracy of the numerical data is of the order of 1%.

L-Tyrosine hydrochloride

Crystals were obtained by treating L-tyrosine with concentrated hydrochloric acid and leaving the solution to evaporate at room temperature. The needle-shaped crystals

were unstable when exposed to air and had to be enclosed in a quartz tube during irradiation.

L-Tyrosine hydrobromide

The crystals were obtained in a manner similar to the hydrochloride. The two compounds were found to be isomorphous.

L-Cystine hydrochloride

Crystals were obtained from a slightly warmed solution of L-cystine in hydrochloric acid, and were found to be unstable. The systematic absences indicate a C -centred lattice, and the space group $C2$ is compatible with the morphological data of Becke (1891), which indicate that the point-group symmetry of the crystal is C_2-2 . The space group has fourfold general positions but the observed number is two. This suggests the presence of diad-axis symmetry in the molecule and indicates that the -S-S- bridges lie across diad axes in the crystal.

The choice of the axes by Becke (1891) is different from ours, but his data agree closely with those reported here. The angle β was determined from goniometric studies.

The cell dimensions for both the cystine compounds agree well with those reported by Steinrauf & Jensen (1956).

Table 1

Compound	Space group	a (Å)	b (Å)	c (Å)	β (°)	Density (g.cm. ⁻³)		Z	Morphology
						Obs.	Calc.		
L-Tyrosine hydrochloride	$P2_1$	11.03	9.10	5.00	90.7	1.42	1.44	2	Needles along [001] bounded by the form {011}
L-Tyrosine hydrobromide	$P2_1$	11.41	9.11	5.17	91.0	1.64	1.62	2	Needles along [001] bounded by the form {011}
L-Cystine hydrochloride	$C2$	18.63	5.26	7.28	103.7	1.52	1.50	2	Needles along [010] bounded by the form {101}
L-Cystine hydrobromide	$P2_12_1$	17.91	5.35	7.48	—	1.87	1.86	2	Needles along [010] bounded by the form {101}
L-Lysine monohydrochloride dihydrate	$P2_1$	7.48	13.31	5.85	97.8	1.25	1.26	2	Slightly elongated along [001] showing faces (010), (110), (110)