

proved by heating a zirconium 'getter' to 1200° C. before heating the uranium. Even then, the most prominent powder lines were those of UO (Rundle, Baenziger, Wilson & McDonald, 1948).

Beta-uranium produces an X-ray diagram similar to, but even more complex than, alpha-uranium. With the powder data available we have thus far been unable to determine the structure or lattice. In view of the similarity of the low-order reflections it seems likely that the beta and alpha structures are related.

At 800° C. the lattice constant for gamma-uranium is 3.48 kX. This value has been obtained from Debye-Scherrer diagrams which did not extend to the back-reflection region, and lacks precision. Similar results have been obtained at Battelle Memorial Institute (1944).

The lattice constant of gamma-uranium at room temperature has been studied as a function of molybdenum content, using a symmetrical, self-focusing, powder camera of 5 cm. radius (Table 1). Graphical extrapolation to pure uranium leads to a lattice constant of 3.467 ± 0.005 kX. and a room-temperature density of 18.89 ± 0.05 g.cm.⁻³, slightly less than that of alpha-uranium at the same temperature. In this extrapolation Vegard's law was assumed, but it is probable that this holds very well, since the data of Table 1 can also be extrapolated to give a reasonably accurate value for the lattice constant of pure molybdenum.

McLennan & McKay (1930) reported a lattice constant for uranium at room temperature of 3.43 kX. It seems

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Extra reflexions from NaClO₃ single crystals. By R. K. SEN. *X-ray Laboratory, Indian Association for the Cultivation of Science, 210 Bowbazar Street, Calcutta, India*

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In a recent communication Garrido (1948) has given the shapes of the iso-diffusion surfaces around the reciprocal-lattice points (120) and (200) of NaClO₃. NaClO₃ is a cubic crystal and its elastic constants are also known. It is therefore possible to map out the iso-diffusion surfaces around the reciprocal-lattice points of this crystal from the expressions of Jahn (1942) so far as the regions very near these points are concerned. In the present communication an attempt has been made to determine the shape of the iso-diffusion surface around the (200) reciprocal-lattice point of NaClO₃ from the theoretical expressions of Jahn, using the values of the elastic constants given by Bhagavantam & Suryanarayana (1947). The surface obtained from Jahn's formulae has also been compared with the experimentally determined surface of Garrido. It has been observed that there are striking differences between the shapes of the theoretical and experimental iso-diffusion surfaces. For, according to Jahn, the intensity of the scattered X-radiation, I , at any point very near a reciprocal-lattice point is given by the expression

$$I \propto \frac{R^2}{r^2} \{c_{44}^2 + \Sigma [L^2 \{c_{44}(c_{11} - c_{44}) (m^2 + n^2) + (c_{11} + c_{12})(c_{11} - c_{12} - 2c_{44}) m^2 n^2\} - 2\Sigma MNmn(c_{12} + c_{44}) [c_{44} + (c_{11} - c_{12} - 2c_{44}) l^2] \} \div \{c_{11}c_{44}^2 + c_{44}(c_{11} + c_{12})(c_{11} - c_{12} - 2c_{44})(l^2 m^2 + m^2 n^2 + n^2 l^2) + (c_{11} + 2c_{12} + c_{44})(c_{11} - c_{12} - 2c_{44})^2 l^2 m^2 n^2\}, \quad (1)$$

Table 1. *Lattice constant of gamma-uranium as function of molybdenum content*

A_0 for U (kX.)	Atomic % of Mo
3.412 ± 0.001	17.3
3.394 ± 0.001	22.8
3.385 ± 0.001	24.2
3.376 ± 0.001	29.4
3.365 ± 0.001	31.2

clear that they obtained the gamma form by the accidental influence of some impurity. It is now known that several metals, including chromium and molybdenum, depress the uranium transitions considerably.

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where R , L , M , N are the radius vector and the direction cosines of the nearest reciprocal-lattice point; r is the distance of the point under consideration from the reciprocal-lattice point in question; l , m , n are the direction cosines of the point of observation; and c_{11} , c_{12} , c_{44} are the elastic constants.

In the case of the (200) reciprocal-lattice point,

$$L = 1, M = 0, N = 0, l = 0$$

and

$$m^2 + n^2 = 1$$

for points of observation lying on a plane parallel to b^* , c^* , and we have

$$I \propto \frac{R^2 \{c_{44}^2 + c_{44}(c_{11} - c_{44}) + (c_{11} + c_{12})(c_{11} - c_{12} - 2c_{44}) m^2 n^2\}}{r^2 \{c_{11}c_{44}^2 + c_{44}(c_{11} + c_{12})(c_{11} - c_{12} - 2c_{44}) m^2 n^2\}},$$

or

$$I \propto \frac{R^2 \{c_{11}c_{44} + (c_{11} + c_{12})(c_{11} - c_{12} - 2c_{44}) m^2 n^2\}}{r^2 c_{44} \{c_{11}c_{44} + (c_{11} + c_{12})(c_{11} - c_{12} - 2c_{44}) m^2 n^2\}},$$

or

$$r^2 \propto \frac{R^2}{I c_{44}},$$

$$\propto \frac{4}{6.57^2 I c_{44}}$$

(since R for the (200) reciprocal-lattice point of NaClO₃ is $2/6.57 \text{ \AA}^{-1}$),

or $r^2 = \text{constant}$ for a constant value of the intensity, I .

Thus the equi-intensity lines around the (200) reciprocal-lattice point in the plane parallel to (b^*, c^*) are circles. But the intersections of the iso-diffusion surface obtained by Garrido around the (200) reciprocal-lattice point by a plane parallel to b^*, c^* are not circles; they are of the form shown in Fig. 1.

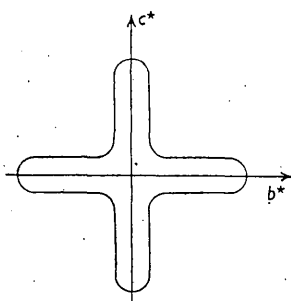


Fig. 1. Section of iso-diffusion surface around (200) reciprocal-lattice point by a plane parallel to b^*, c^* as observed by Garrido.

The section of the iso-diffusion surface by a plane parallel to a^*, b^* as observed by Garrido is of the form shown in Fig. 2 (a). The corresponding iso-diffusion lines obtained from Jahn's formula are shown in Fig. 2 (b). In this case the discrepancy between the theoretical and the experimentally observed iso-diffusion surfaces is not so prominent, but there is no appreciable agreement.

In view of the above discrepancies between theoretical and experimental results, it is natural to conclude that the extra reflexions from NaClO_3 crystals do not owe their origin to the thermal vibrations. In order to ascertain the origin of the extra reflexions in this case a thorough re-investigation of the problem is desirable. Laue photo-

graphs of NaClO_3 at very low temperature will also provide valuable informations in this matter.

It has also been observed that the disagreement between the experimental and the theoretical sections of the iso-diffusion surface by a plane parallel to a^*, b^* is even greater when Voigt's (1910) values of the elastic constants

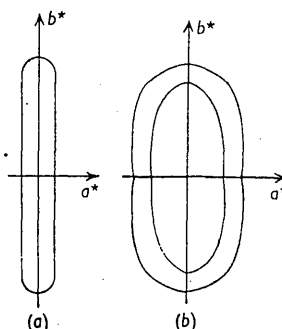


Fig. 2. Section of iso-diffusion surface around (200) reciprocal-lattice point by a plane parallel to a^*, b^* ; (a) as observed by Garrido, (b) as given by equation (1).

are used. The iso-diffusion surfaces obtained from Jahn's formula, using the values of elastic constants of Mason (1946) and of Bhagavantam & Suryanarayana (1947), are almost of the same shape.

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Bifurcated hydrogen bonds. By A. F. WELLS. *Research Laboratories, Imperial Chemical Industries Ltd. (Dyestuffs Division), Hexagon House, Blackley, Manchester 9, England*

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The precise nature of the constitutional differences (if any) between O-H-O bonds of various lengths is not known. The postulation of 'bifurcated' O-H-O bonds in crystals of $\alpha\text{-HIO}_3$ (Rogers & Helmholtz, 1941) further complicates the general picture of the part played by H in intermolecular binding. The object of this note is to point out that there is an alternative and entirely reasonable interpretation of the interatomic distances in this crystal which obviates the necessity for assuming the existence of bifurcated H bonds. The facts are as follows. Crystals of $\alpha\text{-HIO}_3$ are orthorhombic (space group $P2_12_12_1$) with four molecules in the unit cell. There are therefore three sets of non-equivalent O atoms (O_1 , O_2 and O_3). The nearest neighbours of atoms are as follows:

I: 3 O (at 1.80, 1.81, 1.89 Å.) forming a pyramidal IO_3 group;

3 more O (at 2.45, 2.70, 2.90 Å.) completing a distorted octahedral group;

O_1 : 3 O at 2.78 Å., others at 2.90 Å. or more;

O_2 : 4 O at 2.78 Å., others at 3.10 Å. or more;

O_3 : 3 O at 2.78 Å., others at 2.90 Å. or more.

Two of the nearest O neighbours of any O atom are two belonging to its own IO_3 group, within which O-O is 2.78 Å., the same as the shortest O-O distances between O atoms of different IO_3 groups. Rogers & Helmholtz regard all the latter (four per IO_3 group) as hydrogen bonds, and describe them as bifurcated because there are twice as many such bonds as H atoms available. They are shown as broken lines at the left-hand side of Fig. 1, which is a projection of the structure on (100). They then propose positions for the H atoms, as shown to the right in Fig. 1.

There are reasons for regarding this interpretation of the interatomic distances as unsatisfactory. We have determined the crystal structure of the orthorhombic form of selenious acid, H_2SeO_3 , and find that the hydrogen bonding is very similar to that in Fig. 1. This type of structural scheme is to be expected for an oxy-acid with H:O ratio of 2:3, but not for a H:O ratio of 1:3. The alternative interpretation of the structure of $\alpha\text{-HIO}_3$ is as follows.

Rogers & Helmholtz comment on the shortness of the