The orientation of the molecule in the unit cell is

| | $X_m$ | $Y_m$ | $Z_m$ |
|---|---|---|---|
| $a$ | 55° | 147° | 87° |
| $b$ | 48° | 61° | 57° |
| $c^*$ | 118° | 104° | 33° |

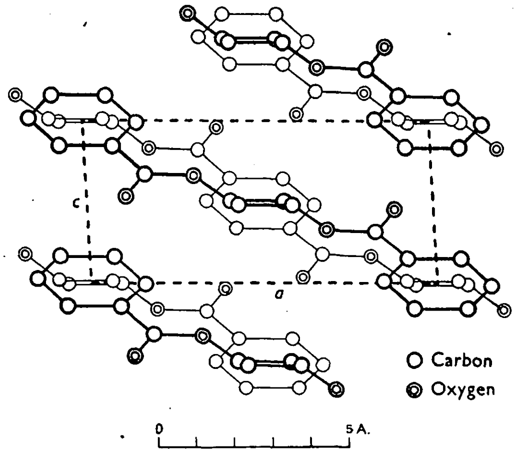

Fig. 5. Diagrammatic projection of the structure on (010).

where $X_m$, $Y_m$, $Z_m$ are three orthogonal axes of the molecule defined by the plane and perpendicular of the benzene ring (Fig. 3). The arrangement is illustrated in Fig. 4. The reason for the (101) cleavage, the large (101) structure amplitude, and the direction of very high refractive index in this plane is shown more clearly in Fig. 5, by the diagrammatic projection of the structure on (010).

The shortest intermolecular contacts are between the $CH_2$ and $CH_3$ groups of one molecule (e.g. with centre at 0, 0, 0) and the ketonic oxygen atoms of the two adjacent space-group-related molecules (centres at $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ and $\frac{1}{2}, \frac{1}{2}, \bar{\frac{1}{2}}$). These distances are 3·47 and 3·48 A. for $C_5$–$O_2$ and 3·41 and 3·49 A. for $C_6$–$O_2$. Other significant intermolecular distances are 3·77 and 3·71 A. respectively between the $C_6$ atom of one molecule (centre, say, 0, 0, 0), and the $C_1$ and $C_2$ atoms of the adjacent molecule (centre 1, 0, 0) and 3·97, 4·00 and 4·25 A. respectively between the same $C_6$ atom and atoms $C_1$, $O_1$ and $C_6$ of the adjacent molecule (centre 1, 0, $\bar{1}$). Since the perpendicular distance between parallel molecules with centres along the $c$ axis is 3·60 A., there can be no distances shorter than this between these molecules. Hence there are only van der Waals forces between molecules.

The structure is one of layers of molecules at intervals of $\frac{1}{2}b$, with the ketonic oxygen to ethyl group contacts between the layers. This accounts for the observed twinning, since, although the relative tilts of molecules in adjacent layers are different in a twinned crystal, these interlayer contacts are still the same.

In conclusion, I wish to thank Dr A. F. Wells and Dr C. J. Brown for their advice throughout the work.

## References

Goodwin, T. H. & Hardy, R. (1938). *Proc. Roy. Soc.* A, **164**, 369.

Jeffrey, G. A. (1947). *Proc. Roy. Soc.* A, **188**, 222.

Robertson, J. M. (1943). *J. Sci. Instrum.* **20**, 169.

Schomaker, V. & O'Gorman, J. M. (1947). *J. Amer. Chem. Soc.* **69**, 2638.

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# Short Communications

*Contributions intended for publication under this heading should be expressly so marked; they should not exceed about* 500 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.*

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## The structures of uranium metal.*

By A. S. Wilson and R. E. Rundle. *Institute for Atomic Research, Iowa State College, Ames, Iowa, U.S.A.*

(*Received* 3 *November* 1948)

Heat-capacity studies first revealed that uranium metal exists in three modifications. X-ray examination has established that the *alpha* phase, stable to 640° C., is the orthorhombic form with the structure reported by Jacobs & Warren (1937). The *beta* phase, stable between 640 and 760° C., is also a phase of low symmetry, but its structure has not yet been determined. *Gamma*-uranium, stable from 760° C. to the melting-point, is body-centered cubic, the structure reported for uranium at room temperature by McLennan & McKay (1930).

X-ray diagrams of *beta*- and *gamma*-uranium at high temperatures, and also at room temperature, have been obtained. The latter can best be obtained by quenching uranium samples containing chromium or molybdenum in solid solution. In our experience, it is impossible to quench pure *beta*- or *gamma*-uranium to room temperature.

Since uranium at high temperature is a good 'getter', elaborate precautions are necessary to obtain satisfactory X-ray data for the *beta*- and *gamma*-ranges. We have accomplished this by sealing uranium wire in evacuated quartz capillaries. Uranium reacts with quartz, so it was necessary to use columbium spacers between quartz and uranium; the vacuum in the quartz capillary was im-

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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 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.

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 |

The authors are indebted to Messrs D. Ahmann, A. Daane and A. Snow for molybdenum alloys, and to Dr H. A. Wilhelm for advice and suggestions.

## References

Battelle Memorial Institute (1944). *Manhattan Project Reports*, CT–2374 and CT–2700.

Jacobs, C. W. & Warren, B. E. (1937). *J. Amer. Chem. Soc.* **59**, 2588.

McLennan, J. C. & McKay, R. W. (1930). *Trans. Roy. Soc. Can.* (3), **24**, 1.

Rundle, R. E., Baenziger, N. C., Wilson, A. S. & McDonald, R. A. (1948). *J. Amer. Chem. Soc.* **70**, 99.

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## Extra reflexions from NaClO$_3$ single crystals.

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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 NaClO$_3$. NaClO$_3$ 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 NaClO$_3$ 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

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

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

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

or

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

or

$$r^2 \propto \frac{R^2}{I} \frac{1}{c_{44}},$$

$$\propto \frac{4}{6{\cdot}57^2} \frac{1}{I\,.\,c_{44}}$$

(since $R$ for the (200) reciprocal-lattice point of NaClO$_3$ is $2/6{\cdot}57\ A^{-1}$),

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