bond length of 1·0 ± 0·1 A., and a C–O–H bond angle of 120 ± 10°. However, no comparable maximum occurs in the region between adjacent carboxyl groups. It is possible, although improbable, that a real maximum has been obscured by the assumption of incorrect temperature-factor parameters for adjacent oxygen atoms. This possibility will be investigated by extending the range of measurement to higher values of sin θ/λ.

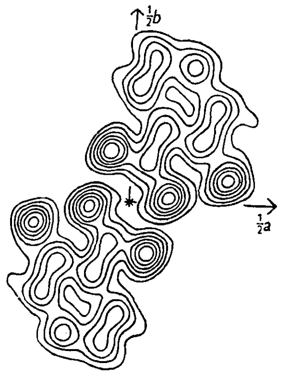

Fig. 1. Electron density projected on (001).

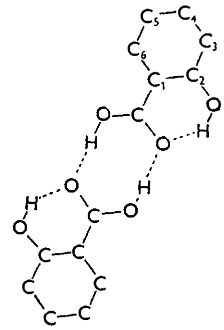

Fig. 2. Pauling's predicted molecular structure.

The above results provide confirmation of Pauling's prediction of the molecular structure shown in Fig. 2 (Pauling, 1945).

A number of the Fourier syntheses used in the course of this work were evaluated on XRAC, the automatic computer designed by Prof. R. Pepinsky and constructed in his laboratory. I am indebted to Prof. Pepinsky for making this possible, and to the Rockefeller Foundation for a grant which has enabled me to work at State College.

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The crystal structure of tetragonal barium titanate.

By Howard T. Evans, Jr., *Philips Laboratories, Inc., Irvington-on-Hudson, N.Y., U.S.A.*

(*Received* 21 *March* 1951)

A detailed crystal structure study of tetragonal barium titanate has been carried out with diffraction intensities measured at room temperature. Integrated intensities have been measured on a single untwinned crystal 0·16 × 0·19 × 0·07 mm., using a Weissenberg camera on which has been mounted a Geiger counter. Ninety-nine reflections ($h0l$) have been measured using Mo $K\alpha$ radiation. Intensities have been corrected by analytical methods for absorption and secondary extinction. The best fit of calculated and observed intensities was obtained with the following structure:

Space group: $P4mm$
Ba in (a): 0, 0, 0.
Ti in (b): $\frac{1}{2}, \frac{1}{2}, (\frac{1}{2}+z_{\mathrm{Ti}})$, $z_{\mathrm{Ti}} = 0{\cdot}015$.
$\mathrm{O_I}$ in (b): $\frac{1}{2}, \frac{1}{2}, z_{\mathrm{O_I}}$, $z_{\mathrm{O_I}} = -0{\cdot}024$.
$2\mathrm{O_{II}}$ in (c): $\frac{1}{2}, 0, (\frac{1}{2}+z_{\mathrm{O_{II}}})$;
$0, \frac{1}{2}, (\frac{1}{2}+z_{\mathrm{O_{II}}})$, $z_{\mathrm{O_{II}}} = -0{\cdot}020$.

This structure gave a ratio of sum of absolute deviations of calculated and observed structure factors to sum of calculated structure factors of 5·71 %. A temperature correction was applied to the calculated values for which the coefficient $B = 0{\cdot}30 \times 10^{-16}$ cm.^{2}. The structure given above is in approximate agreement with the partial solution of the structure given by Kaenzig (1950).

Interatomic distances are as follows:

Ti–$\mathrm{O_I}$ above	1·860 A.	Ba–4$\mathrm{O_I}$	2·826 A.
$\mathrm{O_I}$ below	2·174	–4$\mathrm{O_{II}}$ above	2·782
4$\mathrm{O_{II}}$	2·002	–4$\mathrm{O_{II}}$ below	2·896
$\mathrm{O_I}$–4$\mathrm{O_{II}}$ above	2·850	$\mathrm{O_I}$–$\mathrm{O_I}$	2·824
4$\mathrm{O_{II}}$ below	2·827		

A shift of 0·005 A. of any atom makes the agreement between calculated and observed structure factors significantly poorer.

A detailed description of the work leading to these results will be published shortly.

Reference

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A cubic structure for the phase Pt_3Cu.*

By You-Chi Tang, *Gates and Crellin Chemical Laboratories, Pasadena, California, U.S.A.*

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Schneider & Esch (1944) proposed for the intermetallic phase with composition about Pt_3Cu an orthorhombic structure which is derived from a face-centered cubic arrangement. They found that this structure gave satisfactory agreement with X-ray intensities on their powder photographs, and that no other well-defined arrangement of the atoms gave as good agreement. However, the proposed structure for Pt_3Cu may well not be the right one, inasmuch as an orthorhombic structure such as this would very probably distort the cubic lattice perceptibly; yet no splitting of the diffraction lines was observed.

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* Contribution no. 1527 from the Gates and Crellin Laboratories of Chemistry, California Institute of Technology.