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.

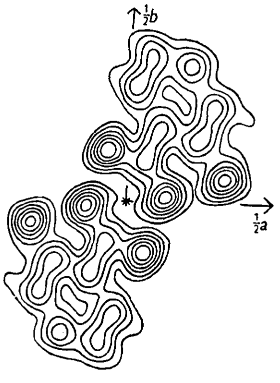

Fig. 1. Electron density projected on (001).

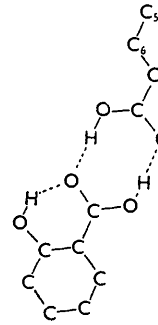

Fig. 2. Pauling's predicted molecular structure.

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.*

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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.

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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.

I have found (Tang, 1950) that the data for this phase, which covers the composition range 63–88 % of platinum, are compatible with a cubic structure of the type ABC_6 with

A at $(0, 0, 0;\ 0, \frac{1}{2}, \frac{1}{2};\ \frac{1}{2}, 0, \frac{1}{2};\ \frac{1}{2}, \frac{1}{2}, 0) + 0, 0, 0;$
B at $+\frac{1}{2}, 0, 0;$
and C at $+\frac{1}{4}, \frac{1}{4}, 0;\ +0, \frac{1}{4}, \frac{1}{4};\ +\frac{1}{4}, 0, \frac{1}{4};\ +\frac{1}{4}, \frac{1}{4}, \frac{1}{2};$
$+\frac{1}{2}, \frac{1}{4}, \frac{1}{4};\ +\frac{1}{4}, \frac{1}{2}, \frac{1}{4},$

as shown in Fig. 1. The structure factors for the three types of unmixed hkl are:

$F_{hkl} = 4(f_A + f_B + 6f_C)$, if hkl are all multiples of 4, or all even but not divisible by 4;

$F_{hkl} = 4(f_A + f_B - 2f_C)$, if hkl are all even and only one or two of them are divisible by 4;

$F_{hkl} = 4(f_A - f_B)$, if hkl are all odd.

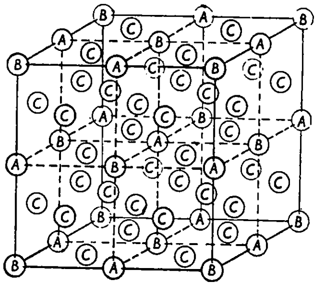

Fig. 1. The cubic structure ABC_6. $Z = 4$.

For the alloy containing 72·5 % of platinum A is Pt, B is Cu and C is the statistical atom $(Pt_{0·8}Cu_{0·2})$. The cubic structure $PtCu(Pt_{0·8}Cu_{0·2})_6$ gives at least as good agreement with X-ray intensities as Schneider & Esch's structure. The calculated intensities and those observed by Schneider & Esch are given in Table 1.

It is not particularly surprising that the alloy in question, which corresponds to a maximum in the electric-conductivity–composition curve and which gave maximum intensities to superstructure lines (Schneider & Esch, 1944) contains the statistical atom $(Pt_{0·8}Cu_{0·2})$. As a matter of fact it is the composition $(Pt_{0·8}Cu_{0·2})Cu_3$ in the cubic phase of nominal composition $PtCu_3$ which corresponds to a high peak in the conductivity diagram and also gives maximum intensities to superstructure lines (Schneider & Esch, 1944; Johansson & Linde, 1927). The statistical atom $(Pt_{0·8}Cu_{0·2})$ may involve some short-range order which is not detectable by ordinary X-ray diffraction methods.

The complex conductivity and X-ray data for the other alloys between 63 and 88 % of platinum in the cubic phase of nominal composition $PtCuPt_6$ are understandable in terms of cubic structures as described by the formula

$$(Pt_{1-x}Cu_x)\ (Pt_yCu_{1-y})\ (Pt_{1-z}Cu_z)_6,$$

where x, y and z are less than 0·3, and $100(7-x+y-6z)/8$ is the atomic percentage of platinum in an alloy.

Table 1. *Calculated and observed intensities for* $PtCu(Pt_{0·8}Cu_{0·2})_6$

hkl	$\sin\theta$	$PLHF^2 \times 10^{-6}$	I
111	(0·173)	9	—
200	(0·200)	2	—
220	0·284	2	*vvw*
311	0·335	11	*vw*
222	0·347	350	*ms*
400	0·402	200	*mw*
331, 402	0·441	11	*vw*
224	(0·510)	2	—
333, 511	0·528	8	*vw*
440	0·565	250	*s*
531	0·592	10	*vw*
600, 442	(0·600)	2	—
620	(0·632)	2	—
335	0·653	5	*vvw*
622	0·663	410	*vs*
444	0·691	135	*m*
551, 711	0·713	10	*vw*
406	(0·720)	2	—
624	0·749	4	*vvw*
731, 553	0·768	15	*vw*
800	0·798	113	*mw*
733	0·818	6	*vw*
802, 446	0·830	5	*vvw*
228, 660	0·845	3	*vvw*
555, 157	0·864	16	*w*
662	0·870	626	*vs*
840	0·893	680	*vs*
911, 735	0·910	28	*w*
842	(0·917)	7	—
664	(0·938)	4	—
913	0·952	29	*vw*
844	0·978	2110	*vs*

P = polarization factor; L = Lorentz factor; H = multiplicity factor. m = moderate; s = strong; v = very; w = weak.

In view of the fact that there is no detectable splitting of the cubic lines and of the satisfactory agreement with X-ray intensities given by the cubic structure $PtCu(Pt_{0·8}Cu_{0·2})_6$, this structure is probably the correct one for the annealed Pt–Cu alloy containing 72·5 % of platinum, and the cubic phase covering the entire range of 63–88 % of platinum is probably similarly based upon the cubic structure ABC_6.

I wish to thank Prof. Linus Pauling for suggesting this problem to me, and for many helpful discussions.

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Structure studies of the two forms of sodium tripolyphosphate.

By J. J. DYMON and A. J. KING, *Department of Chemistry, Syracuse University, Syracuse 10, New York, U.S.A.*

(*Received* 8 *March* 1951)

Sodium tripolyphosphate, $Na_5P_3O_{10}$, is the only crystalline polyphosphate which has been observed as an intermediate phase in the binary system $Na_3P_3O_9$–$Na_4P_2O_7$. Its existence has been substantiated by a number of