

Table 1

	P ₁			P ₂		
	x	y	z	x	y	z
Coordinates from two-dimensional refinement	0.281	0.379	0.709	0.353	0.293	0.463
Final coordinates	0.2821	0.3791	0.7088	0.3531	0.2932	0.4637
	$ \Delta x $	$ \Delta y $	$ \Delta z $	$ \Delta x $	$ \Delta y $	$ \Delta z $
Atomic shifts (Å)	0.010	0.002	0.001	0.001	0.003	0.005
Back-shifts (Å)	0.001	0.012	0.019	0.008	0.003	0.001

atomic shifts were small, the back-shift correction was not repeated.

Making use of Cruickshank's method, the standard deviation due to inaccuracies in the measured intensities was estimated to be 0.005 Å in the P-P bond length. However, a somewhat higher value, namely 0.01 Å, was assumed because of (a) the more or less systematic errors in the scale factors relating the intensities from different layer lines, (b) the imperfection of the method used for the correction for series termination, and (c) the inaccuracies in the dimensions of the unit cell.

The P-P distance, derived from the final coordinates of Table 1, amounts to 2.35 Å. It is now justified to conclude that this value is significantly larger than the values reported for the P-P bond length in black phosphorus (2.18 Å; Hultgren, Gingrich & Warren, 1935), in P₄ tetrahedra in the vapour phase (2.21 Å; Maxwell, Hendricks & Mosley, 1935) and in P₄S₃ (2.24 Å; van Houten, Vos & Wiegers, 1955; Leung, Waser & Roberts, 1955).

The three-dimensional Fourier syntheses were calculated on punched-card machines. We wish to express

our gratitude to Theodorus Niemeijer N. V. for generously putting their I.B.M. equipment at our disposal and to Mr M. R. van der Velde for his assistance in operating these machines. We are also indebted to Messrs H. Schürer and H. A. Tasman for their help in the computational work.

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Structures of the compounds Th₂Cu, ThCu₂, Th₂Zn and ThHg₃.* By N. C. BAENZIGER, R. E. RUNDLE and A. I. SNOW, *Institute for Atomic Research and Department of Chemistry, Iowa State College, Ames, Iowa, U. S. A.*

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Present interest in thorium alloys prompts us to make available crystallographic data on compounds of thorium with copper, zinc and mercury. These have all been obtained from powder diagrams, and in none of these systems were our data on the systems exhaustive.

There are at least three compounds in the thorium-copper system: Th₂Cu, ThCu₂, and probably ThCu₄. We have examined only the first two.

Th₂Cu

Th₂Cu is *b.c.* tetragonal, $a = 7.28$, $c = 5.74$ Å, with the CuAl₂ (Type C16) structure:

4 Cu at $(0, 0, \frac{1}{4}; 0, 0, \frac{3}{4}; \frac{1}{2}, \frac{1}{2}, \frac{1}{4}; \frac{1}{2}, \frac{1}{2}, \frac{3}{4})$;
 8 Th at $0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \pm (x, \frac{1}{2} + x, 0; \frac{1}{2} + x, \bar{x}, 0)$ with $x = \frac{1}{8}$.

The structure has been verified by comparing observed and calculated intensities for powder diagrams. The agreement is very satisfactory.

ThCu₂

ThCu₂ is hexagonal, $a = 4.35$, $c = 3.47$ Å, with the AlB₂ (Type C32) structure:

Th at 0, 0, 0;

2 Cu at $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}; \frac{2}{3}, \frac{1}{3}, \frac{1}{2}$.

Observed and calculated intensities agree well for this structure.

Other data on the thorium-copper system are available from the work of Grube & Botzenhardt (1942), and of Raub & Engel (1943), but the composition of compounds reported by the latter are inaccurate.

* Contribution No. 398: work performed in the Ames Laboratory of the Atomic Energy Commission.

Th₂Zn

This compound is isomorphous with Th₂Cu (see above) with tetragonal lattice constants: $a = 7.60$, $c = 5.64$ Å. Again, calculated and observed intensities confirm the Type C16 structure, with an ideal parameter of $\frac{1}{6}$. (Intensities were also calculated for $x = 0.159$ with no improvement.)

Nowotny (1946) has examined the zinc-rich side of the system, reporting crystallographic data for ThZn₉, and he has discovered another compound richer in thorium, but presumably not Th₂Zn.

ThHg₃

At approximately the composition ThHg₃ a hexagonal phase, $a = 3.38$, $c = 4.72$ Å, occurs with $z = \frac{1}{2}$. Intensity

data are compatible with a disordered hexagonal closest-packed structure, but probably do not exclude ordering. The lattice constants vary somewhat from sample to sample and presumably the composition is variable over a range, but the solubility limits have not been established. The compound resembles UHg₃ (Rundle & Wilson, 1949).

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

Acta Crystallographica: important notice

In order to reduce the pressure of work on the Editorial Board, the Commission on *Acta Crystallographica* has co-opted two additional members. As from 1 January 1956, Prof. E. W. HUGHES (Gates and Crellin Laboratories, California Institute of Technology, Pasadena, Cali-

fornia, U.S.A.) will act as an additional American Co-editor and Prof. H. LIPSON (Physics Department, College of Technology, Manchester 1, England) as an additional British Co-editor. Articles in English should, therefore, be submitted to R. C. Evans, I. Fankuchen, E. W. Hughes, H. Lipson or I. Nitta.

Book Reviews

Works intended for notice in this column should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 99 Livingston Street, Brooklyn 2, N.Y., U.S.A.). As far as practicable books will be reviewed in a country different from that of publication.

Untersuchungen über die Elektronentheorie der Kristalle. By S. I. PEKAR. (Translated from the Russian by H. Vogel.) Pp. viii+184. Berlin: Akademie-Verlag. 1954. Price DM. 13; \$5.85.

The Russian version of this book appeared in 1951 and deals mainly with the theory of polarons as developed by the author and his Russian co-workers from 1944 onwards. A polaron is a particular excited state of an ionic semiconducting crystal in which a free electron, taken from the conduction band, is captured in a potential trough produced by the surrounding ionic charges. Under these circumstances the electron will produce a (radially directed) polarization of the nearby ions and this polarization diminishes the total energy of the state and so helps to keep the electron trapped. Because of its low energy this state in turn diffuses with comparative ease through the crystal. A non-trapped, quickly moving conduction electron cannot produce such polarization because of the inertia of the ions.

The wave-mechanical theory of this complicated state naturally requires many approximations, and there is considerable difference of opinion as to the validity of Pekar's approach in which it is assumed that the potential trough in which the electron is trapped offers energy levels in much smaller steps than those of the normal ions, but that these steps are large compared to those in the infra-red absorption region of the lattice. Thus the trapped electron absorbs photons in a spectral region of transparency of the normal crystal, and the polaron offers a model explanation of *F*-centers. The discussion of *F*-centers is the main object of the second half of the book.

Supplemented by the study of some more recent papers (e.g. H. Fröhlich, *Advances in Phys.* (1954), **3**, 325, R. P. Feynman, *Phys. Rev.* (1955), **97**, 660) this translation gives a good survey of the work done on the polaron. Translator, editor and publisher are to be congratulated on having done a very competent job.

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