Table 1. *Expressions for the structure factors of the unstabilized* Li_3Mg_5 *and the stabilized structure containing interstitial atoms*

(f_I is the atomic scattering factor of the interstitial atom)

Conditions on reflection indices	Unstabilized structure (metal atoms only)	Stabilized structure (metal+interstitial atoms)
$h+k+l \neq 2n$	0	0
$h+k+l = 2n$	—	—
(1) h, k, l mixed	$2(f_{Mg}-f_{Li})$	$2(f_{Mg}-f_{Li})$
(2) h, k, l all even	—	—
(a) $\frac{1}{2}(h+k+l)$ odd	$6(f_{Li}-f_{Mg})$	$6(f_{Li}-f_{Mg})$
(b) $\frac{1}{2}(h+k+l)$ even, $\frac{1}{2}l$ even	$6f_{Li}+10f_{Mg}$	$6f_{Li}+10f_{Mg}+16f_I$
$\frac{1}{2}(h+k+l)$ even, $\frac{1}{2}l$ odd	$6f_{Li}+10f_{Mg}$	$6f_{Li}+10f_{Mg}-16f_I$

It is possible to produce the necessary expansion of the original lattice in the [001] direction by a suitable arrangement of interstitial atoms, but the powder pattern from this stabilized structure differs significantly from that due to the unstabilized structure. The expansion of the [001] direction can be produced by introducing interstitial atoms into the octahedral sites at $(0, 0, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}, 0)$ and symmetry-related positions of the original body-centered cubic cell. In terms of the new cell these positions are:

$$(0, 0, 0; \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2})+$$

4 interstitials in (d): $(0, \frac{1}{2}, \frac{1}{4})$;
4 interstitials in (e): $(0, 0, z)$ with $z = \frac{1}{4}$;
8 interstitials in (h): $(x, y, 0)$, $(\bar{y}, x, 0)$, $(y, \bar{x}, 0)$, $(\bar{x}, \bar{y}, 0)$ with $x = y = \frac{1}{4}$.

If the interstitial atoms are oxygen, then filling of all sixteen sites would increase the [001] dimension from 2×3.5 Å to 9.9 Å, close to the observed 9.7 Å; with nitrogen atoms it would be sufficient to fill only three-quarters of these sites to expand the lattice sufficiently. Again it must be considered highly fortuitous that this expansion is such as to make c/a exactly equal to $\sqrt{2}$.

The expressions for the structure factors of the unstabilized structure of Fig. 1 and that stabilized by sixteen interstitial atoms are given in Table 1. There are five groups of reflections, out of eighteen between Bragg angles for Cu $K\alpha$ of $8°$ and $32°$, for which structure fac-

tors differ significantly; these are the reflections 202; (220, 004); (400, 224); (422, 206) and 044. The bracketed reflections overlap for $c/a = \sqrt{2}$. The interstitial atoms do not contribute to the superstructure reflections, which are therefore the same in both structures.

We have already noted that the uncontaminated structure of Fig. 1 appears to be improbable because of the volume change that would be involved in its formation. This volume change can be accounted for by adding to the unit cell a number of interstitial atoms approximately equal to the number of metal atoms present. The values of the structure factors for the two cells suggest that it would not be too difficult to confuse their powder patterns, especially if quantitative intensity measurements were not made. We conclude that it is improbable that uncontaminated alloys of composition Li_3Mg_5 could have the structure of Fig. 1; the stabilized structure, which cannot be termed an alloy of Li and Mg, is a possible explanation for the observed powder pattern, but its existence must remain essentially speculative until confirmed by density measurements or accurate intensity measurements.

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Refinement of the P–P bond length in P4S7. By AAFJE VOS and E. H. WIEBENGA, *Laboratorium voor Anorganische en Fysische Chemie der Rijksuniversiteit Groningen, Netherlands*

In a recent structure determination of P_4S_7 a remarkably large value, 2.37 Å, for the P–P bond length in the molecule was observed (Vos & Wiebenga, 1955). To this bond length, however, a rather large standard deviation, 0.04 Å, had to be assigned because of overlap in the projections from which the coordinates were derived. It therefore seemed desirable to determine the positions of the two phosphorus atoms concerned (P_1 and P_2) more accurately.

A more reliable value for the P–P bond length has now been obtained by computing the three-dimensional electron-density distribution around P_1 and P_2. The required intensities of the reflexions hkl could be taken

from the original structure determination in which they had been used for the calculation of a three-dimensional Patterson synthesis. The scale and temperature factors were redetermined separately for the different layer lines by comparison with the calculated structure factors. The disagreement index R amounted to 0.13; the best average value for the temperature factor was $\exp(-2.8\sin^2\theta/\lambda^2)$, which is slightly different from the value obtained during the two-dimensional refinement.

For locating the peak maxima an analytical method (Shoemaker, Donohue, Schomaker & Corey, 1950) was used; a back-shift correction for series termination was applied. The results are shown in Table 1. Since the

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 P_4 tetrahedra in the vapour phase (2·21 Å; Maxwell, Hendricks & Mosley, 1935) and in P_4S_3 (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

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Structures of the compounds Th_2Cu, $ThCu_2$, Th_2Zn and $ThHg_3$.*

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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: Th_2Cu, $ThCu_2$ and probably $ThCu_4$. We have examined only the first two.

Th_2Cu

Th_2Cu is *b.c.* tetragonal, $a = 7·28$, $c = 5·74$ Å, with the $CuAl_2$ (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 $x = \frac{1}{6}$.

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

$ThCu_2$

$ThCu_2$ is hexagonal, $a = 4·35$, $c = 3·47$ Å, with the AlB_2 (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.