

The compound appears to be isostructural with  $\text{Pt}_2\text{Ga}_3$  which has the space group  $P\bar{3}m1 (D_{3d}^5)$  of the  $\text{Ni}_2\text{Al}_3$  type. Interplanar spacings and estimated intensities are given in Table 2.

Table 2. Observed interplanar spacings for compound formed at 460 °C on heating 50/50% Pt–Al films in the electron microscope

<i>hkl</i>	<i>d</i>	Intensity
001	5.16 Å	Medium strong
100	3.64	Strong
101	2.98	Strong
102, 110	2.11	Very strong
111	1.95	Medium
200	1.83	Weak
003, 201	1.727	Medium
112	1.635	Very weak
103	1.564	Weak
202	1.492	Medium strong
210	1.382	Weak
113, 211	1.332	Medium strong
203	1.255	Very weak
212, 300, 104	1.218	Medium strong
301	1.187	Very weak
302, 114	1.105	Weak
213	1.078	Weak
204, 220	1.055	Weak

Cell dimensions:  $a = 4.22 \pm 0.01$  Å  
 $c = 5.17 \pm 0.01$   
 $c/a = 1.225$

Probable space group:  $P\bar{3}m1 (D_{3d}^5)$

With more rapid heating of a 50/50% Pt–Al film (about 10°/min) a compound was formed at 410 °C with a crystallite size not exceeding 2  $\mu$ . Also present were small crystallites of  $\text{PtAl}_2$ . From single-crystal patterns of crystals in three different orientations it was determined that the compound was orthorhombic with

$$a = 9.79 \pm 0.04, \quad b = 11.28 \pm 0.05 \quad \text{and} \quad c = 6.58 \pm 0.03 \text{ \AA}.$$

The crystal orientations were (001), (010) and (101). This compound was also formed when 78/22% Pt–Al films were heated to 510 °C and then cooled.

### Discussion

Because of the small size and quantity of the compounds observed, no elementary analysis was obtained. It is

of interest to note that Klemm, Dorn & Huch (1958) reported evidence of a compound existing between 65 and 70 at.% platinum. If one plots a curve of unit cell dimensions *versus* atomic percentage of platinum for the cubic compounds  $\text{Pt}_3\text{Al}$ ,  $\text{PtAl}$  and  $\text{PtAl}_2$  the point for the cubic phase ( $a = 4.10$  Å) found in this investigation falls on the curve at a composition of approximately 66.7% platinum, suggesting the compound  $\text{Pt}_2\text{Al}$ .

Table 3. Comparison of structures of compounds in the systems Pt–Al and Pt–Ga

Compound	Structural type	Cell dimensions	Reference
PtGa	$B20$	$a = 4.90$ Å	Esslinger & Schubert (1957)
PtAl	$B20$	$a = 4.865$ Å	
PtGa <sub>2</sub>	$C1$	$a = 5.923$ Å	Zintl, Harder & Haucke (1937)
PtAl <sub>2</sub>	$C1$	$a = 5.922$ Å	
Pt <sub>2</sub> Ga <sub>3</sub>	$D\bar{5}_{13}$	$a = 4.23$ Å $c = 5.18$ Å $c/a = 1.223$	Hellner & Laves (1947)
Pt <sub>2</sub> Al <sub>3</sub> (?)		$a = 4.22$ Å $c = 5.17$ Å $c/a = 1.225$	

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### An application of Taylor's method for determining the relative positions of molecules. By

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A systematic method of solving the position problem in crystal structure determination, devised by Taylor (1954, 1957) is based upon the principle of the structure-factor graph (Bragg & Lipson, 1936) and has been successfully used on a number of structures.

In the paper describing the basic principle and the theory of the method, Taylor & Morley (1959) pointed

out that the method can be applied in a completely objective way to structures for which both the shape and the orientation of the molecule are exactly known; they felt, however, that it could probably be more useful at an earlier stage of the structure determination, when there is still considerable doubt about the precise shape and orientation of the molecule. It will be shown in the present paper that when applied to the determination of the structure of 4,4'-dihydroxythiobenzophenone monohydrate, Taylor's method proved capable of deter-

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mining the position of the molecule, although its assumed shape and orientation were far from correct. The assumed molecule of the trial structure and the correct one, corresponding to the final coordinates after refinement, are illustrated in Fig. 1.

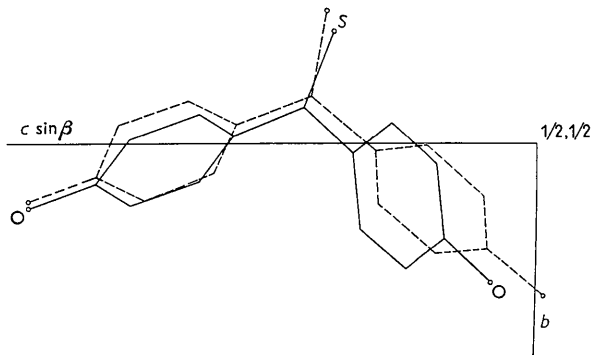
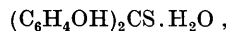


Fig. 1. The assumed molecule of the trial structure (dotted lines) and the correct molecule corresponding to the final data of refinement (continuous lines).

4,4'-Dihydroxythiobenzophenone monohydrate,



crystallizes in the monoclinic space group  $P2_1/c$ , with four molecules in a unit cell of the following dimensions:

$$a = 5.62, b = 10.95, c = 20.24 \text{ \AA}; \beta = 103.5^\circ.$$

All the work to be described has been carried out on the [100] projection, which belongs to the plane group  $pgg$ . The molecular location method was applied in conjunction with optical-transform methods (Hanson, Lipson & Taylor, 1953).

An examination of the  $0kl$  section of the weighted reciprocal lattice, reproduced in Fig. 2, suggested that the long axis of the molecule is roughly parallel to the  $c \sin \beta$  direction. However, owing to the presence of two non-parallel sets of four benzene rings in the unit cell, it proved impossible to deduce the tilt and the orientation

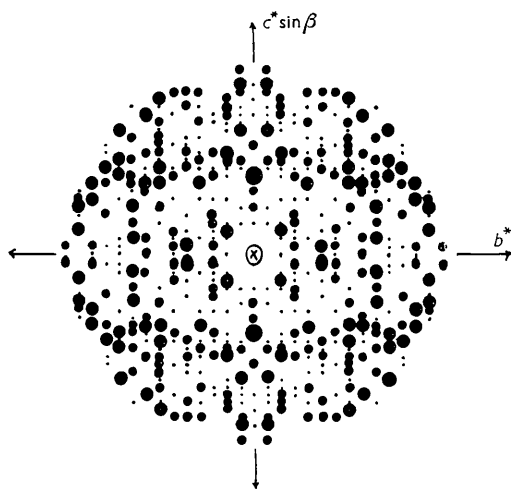


Fig. 2. The  $0kl$  section of the weighted reciprocal lattice.

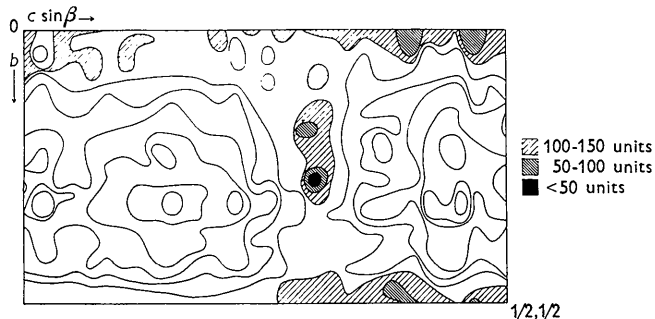


Fig. 3. Graph of the function  $\Sigma ||G(k, l) - |F_o(k, l)||$ . Contours are drawn at intervals of 50 units.

of the benzene rings from the weighted reciprocal lattice. A number of optical transforms of the single molecule, with different shapes and orientations, were made and the molecule whose transform showed the best resemblance to the weighted reciprocal lattice was taken for further consideration.

To find the position of the molecule in the unit cell Taylor's method was applied. Eight reflexions of zero intensity and lying on the strong parts of the optical transform of the single molecule were chosen and the sum of functions  $||G(k, l) - |F_o(k, l)||$  for these reflexions was calculated. The computation was performed by means of Beevers-Lipson strips (Lipson & Beevers, 1936) following the procedure described by Taylor & Morley (1959). The graph of the resulting summation is presented in Fig. 3. It can be seen that there is only one small region where the function has a value less than 50 units and this pronounced minimum was taken as the position of the molecule. An optical transform of the arrangement thus found was prepared and it showed some agreement with the weighted reciprocal lattice; at this stage the agreement residual was calculated to be 64% for all reflexions. The refinement was carried on by the computational methods, and at the point when the residual factor for 80% of observed reflexions, with  $F_o \neq 0$ , had a value of 31%, the shape of the molecule was considerably corrected; further refinement has brought the residual down to 9.5% for all reflexions.

Full details of the structure of 4,4'-dihydroxythiobenzophenone monohydrate will be published elsewhere.

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