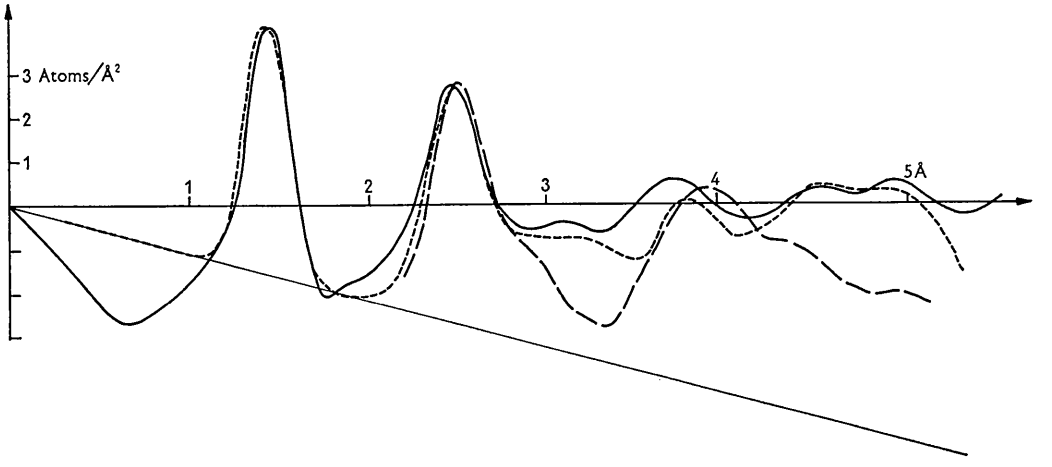

Fig. 1. Experimental and calculated σ/r-curves. Full line: Experimental curve. Dotted: Calculated for three-dimensional network. Broken: Calculated for turbostratic packing of graphite layers. Straight line: *minus* the even distribution $4\pi\varrho_{\text{atomic}}/r$.

The peaks were approximated by Gaussian curves, and the half widths were taken as a descending function of r.

It has to be mentioned that good agreement with the experimental radial distribution appears to be achievable also for the other three-dimensional networks containing 7-rings or other types of 8-rings. It does not seem justified from the present data, however, to make any discrimination between these models and the one considered here. In any case, the structure is very likely to contain a great number of irregularities and very little long-range order as also suggested by Blue & Danielson (1957) from measurements of electrical properties. It should perhaps be noted that films produced during one of the evaporation experiments rendered diffractograms displaying more pronounced halos than usual. A radial distribution curve calculated from these diffractograms indicated a faint split of the nearest-neighbor peak whereas the remaining features did not differ appreciably from the other curves.

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Crystallographic data for 5-oxiphenazine.

By R. CURTI and V. RIGANTI, *Department of General Chemistry, Pavia University, Pavia, Italy*

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5-oxiphenazine is a yellow substance, which melts at 226·5 °C. and is obtainable as single crystals from ethylmethylketone. The crystals used in this study were obtained from a sample prepared by Mr S. Locchi, using the method of Wohl & Aue (1901). These were small needles elongated along *b*, bounded on the sides by prominent {100} and {102}, and small {001} faces, and on the ends by {011} and {111} faces. Although most of the crystals were poorly formed, and some faces occurred as curved surfaces, a few suitable for goniometric measurements for single-crystal X-ray photographs were found.

By goniometric measurements the following constants were determined: crystal system: monoclinic; axial angle: $\beta = 108° 52'$; axial ratios: $a:b:c = 1{\cdot}632:1:3{\cdot}115$. Rotation, equi-inclination Weissenberg and precession photographs were taken, using Cu $K\alpha$ radiation. The cell dimensions were determined from the rotation and zero-level Weissenberg photographs, the camera radius of

57·162 mm. having been determinated by calibration with sodium chloride. The dimensions of the unit cell were found to be:

$$a_0 = 7{\cdot}37 \pm 0{\cdot}02,\ b_0 = 4{\cdot}60 \pm 0{\cdot}02,\ c_0 = 14{\cdot}34 \pm 0{\cdot}03\ \text{Å};$$
$$\beta = 108°\ 59' \pm 8'.$$

These data give the axial ratios: $a:b:c = 1{\cdot}602:1:3{\cdot}118$.

The observed density of 1·42 g.cm.$^{-3}$ agrees well with the density of 1·417 g.cm.$^{-3}$ calculated on the basis of two formula units per unit cell.

When the diffraction spots in the Weissenberg and precession photographs were indexed the following interferences were observed: hkl in all orders; $h0l$ when $l = 2n$; $0k0$ when $k = 2n$. These data are consistent with the space group C_{2h}^5–$P2_1/c$. Structural investigations on 5-oxiphenazine and 5-10-dioxiphenazine are in progress.

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The crystal structure of Zr_4Al_3.

By C. G. WILSON, D. K. THOMAS and F. J. SPOONER, *Royal Military College of Science, Shrivenham, Berks, England*

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The crystal structure of the intermetallic compound Zr_4Al_3 has been determined from powder photographs. Powder specimens were obtained by filing from a solid sample of the alloy prepared by arc melting in argon by Miss J. Murray, A.E.R.E., Harwell. Microscopic examination of a polished surface of the solid sample shewed it to be mainly single phase. The photographs obtained with a precision 19 cm. camera (Adam, 1954) gave fairly broad lines with a heavy background caused by the Zr $K\alpha$ radiation excited by the continuous spectrum of the Cu target. Whilst these photographs enabled a unit cell to be determined, more accurate measurements of line spacings and intensities were made on a photograph taken by Dr J. Adam with a focusing camera using monochromatised Cu $K\alpha$ radiation. An attempt was made to find single crystals of suitable size in a crushed specimen, but this proved impossible. The values of $\sin^2\theta$ obtained from measurements made with a Cambridge universal measuring machine and the visual estimate of line intensities is given in Table 1.

Table 1. *X-ray data*

(hkl)	$\sin^2\theta$ (obs.)	$\sin^2\theta$ (calc.)	Intensities (obs.)	Intensities (calc.)
0001	0·0204	0·0204	*m*	2·3
$10\bar{1}0$	0·0268	0·0268	*m*	2·7
$10\bar{1}1$	0·0472	0·0473	*m*	2·9
$11\bar{2}0$	0·0805	0·0805	*vs*	18·4
0002	0·0817	0·0818	*vvw*	0·4
$11\bar{2}1$	0·1009	0·1010	*vs*	10·3
$20\bar{2}0$	0·1073	0·1074	*ms*	3·1
$10\bar{1}2$	0·1086	0·1086	*vs*	19·0
$20\bar{2}1$	0·1277	0·1278	*ms*	4·9
$20\bar{2}2$	0·1887	0·1888	*m*	3·3
$21\bar{3}1$	0·2079	0·2080	*vw*	0·6
$10\bar{1}3$	0·2104	0·2105	*vvw*	0·3
$30\bar{3}0$	0·2412	0·2412	*m*	3·4
$30\bar{3}1$	0·2615	0·2616	*m*	2·3
$11\bar{2}3$	0·2640	0·2614	*m*	2·2
$21\bar{3}2$	0·2692	0·2692	*s*	8·9
$20\bar{2}3$	0·2909	0·2909	*w*	1·3
$22\bar{4}0$	0·3216	0·3216	*m*	3·6
0004	0·3267	0·3266	*vw*	1·2
$22\bar{4}1$	0·3422	0·3420	*vvw*	0·3
$31\bar{4}1$	0·3684	0·3688	*vvw*	0·2
$21\bar{3}3$	0·3711	0·3713	*vvw*	0·2
$22\bar{4}2$	0·4034	0·4032	*vvvw*	0·16
$11\bar{2}4$	0·4071	0·4070	*m*	2·9
$30\bar{3}3$	0·4250	0·4249	*vw*	1·0
$31\bar{4}2$	0·4302	0·4299	*ms*	4·1
$20\bar{2}4$	0·4339	0·4336	*vvw*	0·6
$40\bar{4}1$	0·4490	0·4492	*vvw*	0·7
$40\bar{4}2$ / 0005	0·5105	0·5104 / 0·5105	*w*	0·8
$31\bar{4}3$	0·5323	0·5321	*vvvw*	0·16

vs = very strong; *s* = strong; *ms* = medium strong; *m* = medium; *w* = weak; *vw* = very weak; *vvw* = very very weak; *vvvw* = extremely weak.

Several weak and very weak lines appearing on the focusing camera film have been shown to belong to a neighbouring phase in the Zr–Al system. All the remaining lines have been indexed on a hexagonal unit cell with:

$$a = 5{\cdot}433 \pm 0{\cdot}002,\ c = 5{\cdot}390 \pm 0{\cdot}002\ \text{Å}.$$

Assuming that the volumes occupied by the individual atoms in the alloy are not appreciably different from those occupied by these atoms in the elements, the number of formula units of Zr_4Al_3 per unit cell is unity. On this basis the calculated density is 5·37 g.cm.$^{-3}$. The density of the solid sample determined using a specific-gravity bottle was 5·28 g.cm.$^{-3}$.

No systematic absences were observed and packing considerations led to a choice of space group C_{3h}^1–$P\bar{6}$. The calculated line intensities shown in Table 1 are obtained with the atoms in the following positions:

3 Al 2(j) $x, y, 0$; with $x = \frac{1}{3}$, $y = \frac{1}{6}$.
2 Zr 3(h) $\frac{1}{3}, \frac{2}{3}, z$; with $z = \frac{1}{4}$.
1 Zr $\bar{6}$(f) $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$.
1 Zr $\bar{6}$(b) $0, 0, \frac{1}{2}$.

The interatomic distances are as follows:

(6) Al–Zr 3·03 Å
(6) Zr–Zr 3·41
(1) Zr–Zr 2·70
(2) Al–Al 2·72