by replacing 2U atoms with 2Ir atoms and removing 2C atoms. The structure parameters are compared in Table 2. Interatomic distances between nearest neighbors are listed in Table 3.

Table 2. *Comparison of* UC *and* U_2IrC_2

Space group $I4/mmm$

6UC	$2U_2IrC_2$
$a=a_c/\sqrt{2}=$ 3·51	$a=$ 3·480
$c=3a_c$ =14·88	$c=$12·482
2U in 2(*a*) (000)	2Ir in 2(*a*)
4U in 4(*e*) (00*z*)	4U in 4(*e*)
$z=\frac{1}{3}$	$z=0{\cdot}355$
2C in 2(*b*) (00$\frac{1}{2}$)	—
4C in 4(*e*) (00*z*)	4C in 4(*e*)
$z=\frac{1}{6}$	$z=0{\cdot}168$

Table 3. *Interatomic distances*

U–1C	2·335 (27)
U–4C	2·477 (3)
U–4Ir	3·056 (9)
U–4U	3·480 (1)
Ir–2C	2·093 (22)
Ir–8U	3·056 (9)
C–1Ir	2·093 (22)
C–1U	2·335 (27)
C–4U	2·477 (3)

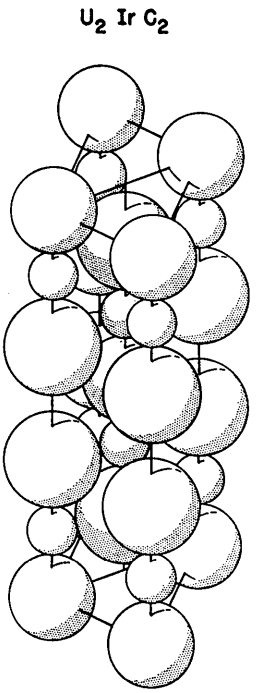

Fig. 2. Pictorial representation of U_2IrC_2.

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The structure of *p*-azoxyanisole.

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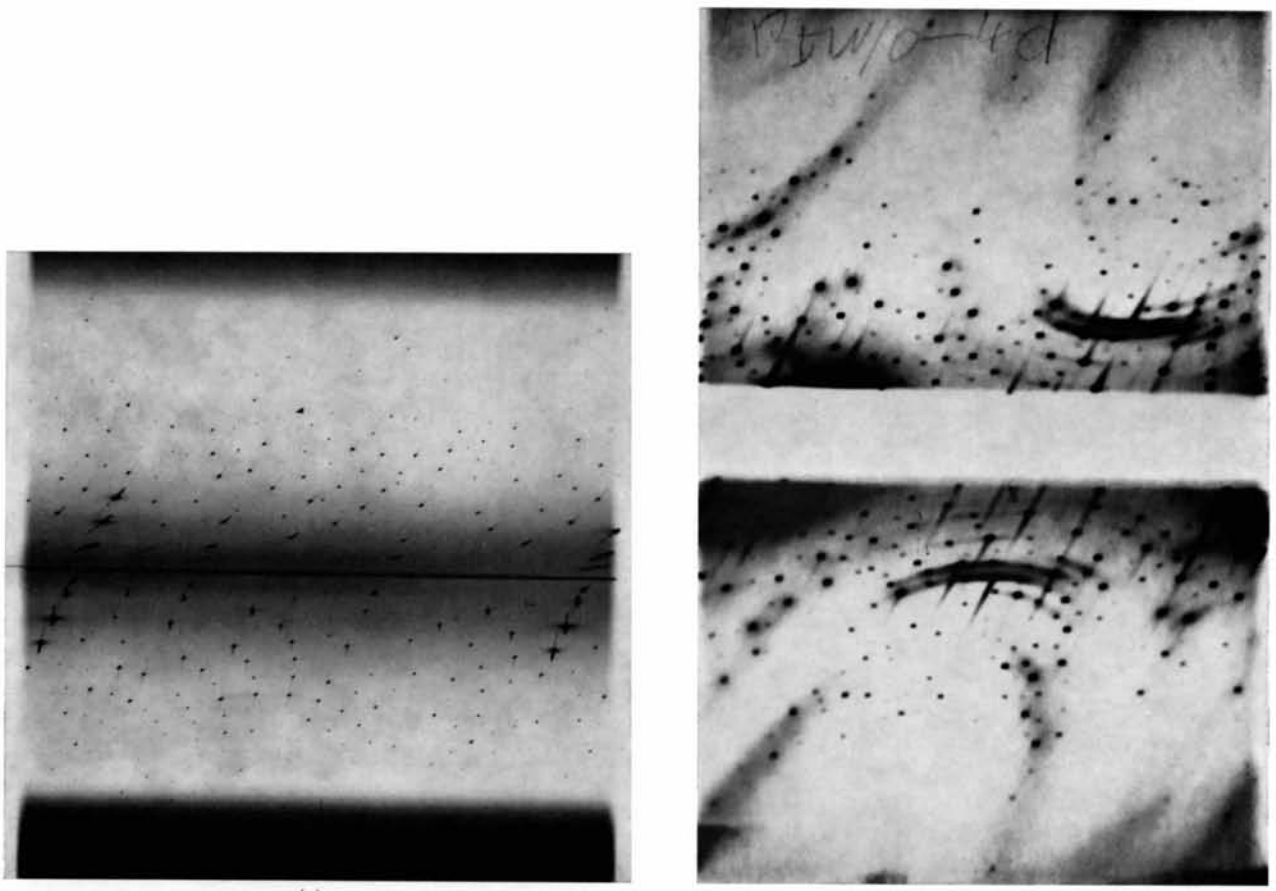
p-Azoxyanisole crystallizes in the monoclinic system. The space group is $P2_1/c$ with $a=1{\cdot}09$, $b=0{\cdot}81$, $c=1{\cdot}56$ nm, $\beta=114°$, and $Z=4$.

It was learned shortly before the International Union of Crystallography meeting in 1969 at which we presented a paper on the crystal structure determination of the liquid crystal *p*-azoxyanisole (Carlisle & Smith, 1969) that Krigbaum, Chatani & Barber (1970), Braun, Hornstra & Leenhouts (1969), and Bednowitz (1970) had also independently and unknown to each other successfully determined the structure of this crystal. The results from all four laboratories are in agreement and this communication sets out very briefly the results obtained by us.

The crystals of *p*-azoxyanisole are monoclinic with $a=1{\cdot}09$, $b=0{\cdot}81$, $c=1{\cdot}56$ nm and $\beta=114°$, space group $P2_1/c$ and $Z=4$.

Data using filtered Cu $K\alpha$ radiation were collected by photographic means in contrast with the other three groups who used diffractometer methods. The intensities of 1006 independent reflexions out of a (theoretically) possible 3000 were visually estimated and used in the investigation. The structure was solved by the symbolic addition method of Karle & Karle (1966) and was refined to an R value of 18·6% using anisotropic temperature factors and no weighting scheme. Fig. 1 shows the projected view of the structure on (010) and Fig. 2 shows the view down the a axis. This R value, which excludes the use of H atoms, compares not unfavourably with the lower R values of 9·1% obtained by Krigbaum *et al.* (1970), of 6·7% obtained by Braun *et al.* (1969) and of 8·1% obtained by Bednowitz (1970), all of whom included the scattering contribution of hydrogen atoms in their final results. A suitable weighting scheme would almost certainly have reduced the R value (18·6%) obtained by us.

The detailed characteristics of the four structures are essentially the same. The atomic coordinates, after transforming axes as necessary, have been compared and the differ-



(a) (b)

Fig. 3 X-ray Weissenberg photographs of (a) $h1l$ reflexions of p-azoxyanisole, (b) $h0l$ reflexions of p-azoxyphenetole, showing smear effects. The enhanced smearing in (b) is partly due to over exposure and to the integration of the intensities of reflexions.

ences appear in most cases at the third significant figure. A noticeable feature is that the four structures have not revealed any marked anisotropy of the atomic vibrations and, furthermore, there is no preferred vibrational direction taken collectively for the ellipsoids.

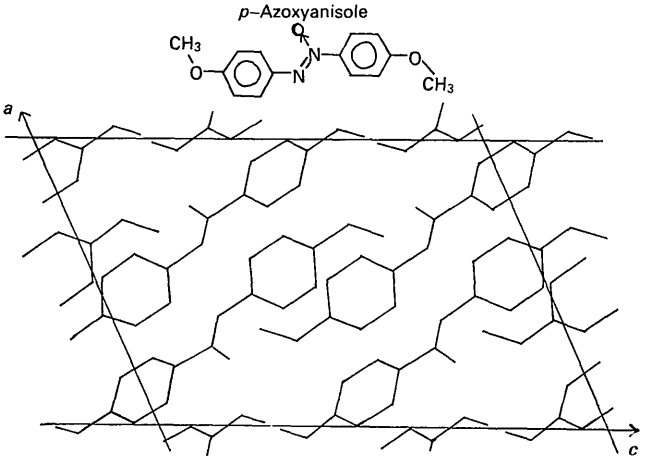


Fig. 1. Projection on (010) of *p*-azoxyanisole molecules.

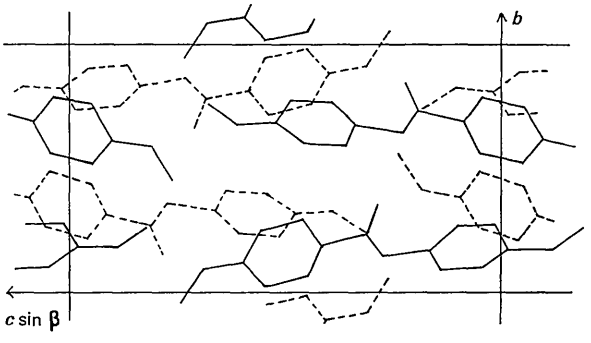


Fig. 2. Projection down the *a* axis of *p*-azoxyanisole.

We undertook this structure determination primarily to see if any light could be thrown on the nature of the mesophases of the material. While the molecules pack in an imbricated manner, as originally pointed out by Bernal & Crowfoot (1933), this observation alone, which has now been confirmed, does not by itself explain why the crystals should go through the nematic phase on heating. At the time of the preparation of our abstract for the I.U.Cr. Congress, it was thought that there was some evidence of disorder in the structure, but further work cast doubts on this view. Furthermore, the low *R* values for the independent structure determinations tend, if anything, to throw less light on this problem. Hence the 'smears' connecting the X-ray reflexions in the X-ray diffraction patterns, as originally noticed by Bernal & Crowfoot and confirmed by us and by Krigbaum *et al.* and by Braun *et al.* need more careful evaluations both from the kinematic and dynamical points of view. We have found this effect to be very marked in the case of our crystals of *p*-azoxyphenetole. Fig. 3(*a*) and (*b*) show for comparison the 'smear' effects observed in the diffraction patterns of the two crystals.

Work is now proceeding on the structure determination of the phenetole compound whose molecules also pack in an imbricated manner, as shown from preliminary investigations (Smith, 1969).

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The water molecules in $AlCl_3.6H_2O$.

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Proton magnetic resonance line shapes of polycrystalline $AlCl_3.6H_2O$ have been fitted with least-squares to a line-shape function containing a variable parameter dependent on the H–H distance of the water molecule. The H–H distance corresponding to the best fit is found to be $1{\cdot}59 \pm 0{\cdot}01$ Å in disagreement with the value 1·70 Å reported by Buchanan & Harris using neutron diffraction.

The structure of aluminum chloride hexahydrate has been studied with X-ray and neutron diffraction techniques by Buchanan & Harris (1968). The dimensions of the hexagonal unit cell were given as a, $c = 11{\cdot}827$, $11{\cdot}895$ Å with $R\bar{3}c$ space group symmetry and $Z = 6$. The six water molecules surround a central aluminum ion forming an essentially regular close-packed octahedron. The two hydrogen atoms associated with a given oxygen atom form normal hydrogen bonds to the nearest-neighbor chlorine ions at 3·02 and 3·03 Å from oxygen. The H–H distance of the water molecule was reported by Buchanan & Harris to be 1·70 Å. This rather high value of the H–H distance attracted our attention.

All thirty-six water molecules in the unit cell of $AlCl_3 \cdot 6H_2O$ are structurally equivalent. This makes $AlCl_3 \cdot 6H_2O$ particularly suitable for a simple proton magnetic resonance (p.m.r.) study in the polycrystalline form. The technique involves fitting the shape of the ob-