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A preliminary X-ray investigation of pristimerin.

By C. H. CARLISLE and M. EHRENBERG, *Crystallography Laboratory, Birkbeck College, London W. C. 1, England*

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A communication by Kulkarni & Shah (1954) describing the preliminary chemical analyses of pristimerin, $C_{28}H_{36-38}O_4$, draws attention to some X-ray work carried out on these crystals at Birkbeck College. It is the purpose of this communication to describe the X-ray investigation in a little more detail.

Two crystalline forms of the substance grown respectively from petroleum ether and acetone were obtained. Their optical and X-ray examinations are summarized in the table below.

	Form *A*	Form *B*
Solvent	Petroleum ether (60–80° C.)	Acetone
Forms	Very small crystals needle-like along [100], with {001}, dominating	Very small crystals lath-like along [001], with {010} dominating; marked pseudo-hexagonal symmetry
Colour	Yellow	Yellow
a (Å)	7·8	15·5
b (Å)	15·6	26·8
c (Å)	41·0	23·25
Density (from salt solution) (g.cm.$^{-3}$)	1·12±0·02	1·08
Number of molecules in unit cell	8	16
X-ray molecular weight	415	393
Space group	$P2_12_12_1$	$C222_1$
Optics	$\alpha \parallel b$ $\beta \parallel a$ $\gamma \parallel c$	$\alpha \parallel c$ $\gamma \parallel a$ $\beta \parallel b$
Dichroism	* { *X* yellow *Y* orange	† { *X* yellow *Y* orange

* On (001). † On (010).

Form *A*

Out of the crop of small crystals it was possible to select one large enough to give the basal reflexions about the *a*, *b* and *c* axes. Those for *b* were obtained with a Weissenberg camera and those for *a* and *c* with a Buerger precession camera, using the same crystal. From this X-ray information the three Patterson projection maps (Fig. 1) along *a*, *b* and *c* were calculated.

As the chemical analysis of this substance is incomplete no light can be thrown on the stereochemical aspects of this molecule in relation to these vector maps. One interesting point does, however, arise from the Patterson vector projection along *c* (see Fig. 1(*c*)); this shows a series of peaks lying parallel to *a* which possibly indicates the presence of flat molecules seen end-on in the crystal. The optical vibrations of the crystal are in agreement with this assumption; the planes of the molecules should

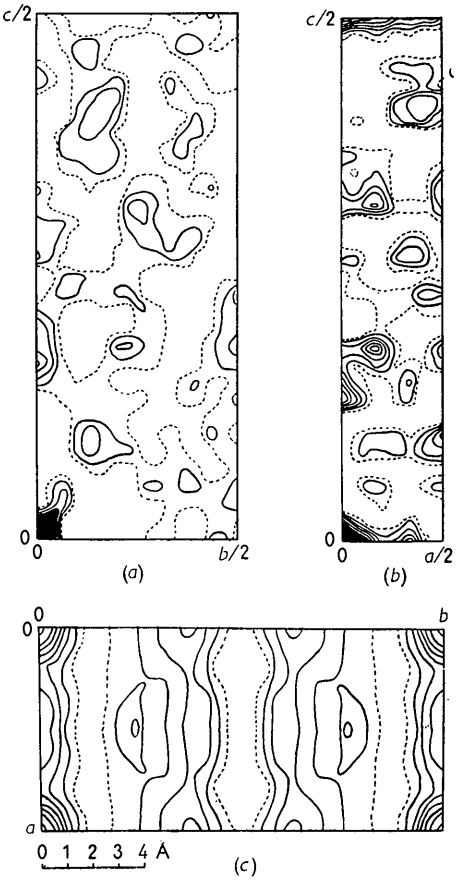

Fig. 1.

be lying nearly parallel to (010). Chemical composition, colour of the crystals and the presence of dichroism suggest that this organic compound is a conjugated system; this would be in keeping with the presence of a quinone ring system already suggested as the basic skeleton for this molecule.

Form *B*

The cell dimensions of this second form suggest a molecule of the same dimensions, so arranged that they are stacked with their molecular planes lying approximately perpendicular to *c*, and with their lengths lying nearly parallel to *b*. No Patterson vector maps have been calculated for this form.

It would appear from these studies that Form *A* is crystallographically more suitable for a detailed investigation.

Reference

KULKARNI, A. B. & SHAH, R. C. (1954). *Nature, Lond.* **173**, 1237.