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# A Simple Adapter for Rotation Cameras to Improve the Accuracy of Measurement of Identity Periods

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(*Received* 4 *October* 1956)

A simple adapter is described which makes it possible to measure identity periods from rotating-crystal photographs with an accuracy of the order of 0·1%.

## Introduction

Identity periods in crystals are related to the separation of layer lines in rotating-crystal photographs by the expression

$$a = n\lambda/\sin \nu_n\,, \tag{1}$$

where $a$ is the identity period and $\nu_n$ the semi-opening cone angle of the $n$th layer (Fig. 1). Differentiation of (1) leads to

$$\Delta a/a = -\cot \nu . \Delta\nu\,, \tag{2}$$

which relates the error in $a$ to the error in the measurement of $\nu$.

For the conventional film mounting in a rotation camera (Fig. 1 (position $A$) and Fig. 2($a$)) two factors limit the accuracy. First, $\nu$ is limited to angles $< 55°$, so that $\cot \nu$ is always $> 0·7$. Secondly, in the terminology of Buerger (1942, p. 95), $\Delta\nu = \cos^2 \nu/r . \Delta y$, where $r$ is the radius of the camera and $\Delta y$ is the error in the measurement of the separation of the layer lines. At the upper limit of $\nu$, $\cos^2 \nu = 0·3$, but, owing to beam divergence and oblique incidence of the diffracted beams on the double-coated film, $\Delta y$ increases about 4–5 times (a value determined from Fig. 2($a$), but representative of typical rotation photographs) and hence $\Delta\nu$ for upper layer lines is slightly greater than for lower layer lines. The expected increase in accuracy for upper layer lines due to the $\cot \nu$ term in (2) is therefore partly reduced by the increase in $\Delta\nu$.

## Principle of the adapter

A film mounting which would permit normal incidence of reflexions in the range $0° < \nu < 90°$, would overcome these disadvantages (Fig. 1 (position $B$)) since the size of reflexions would not vary with $\nu$ for a small crystal of the usual dimensions. $\Delta\nu$ would remain constant and full advantage could be taken of the

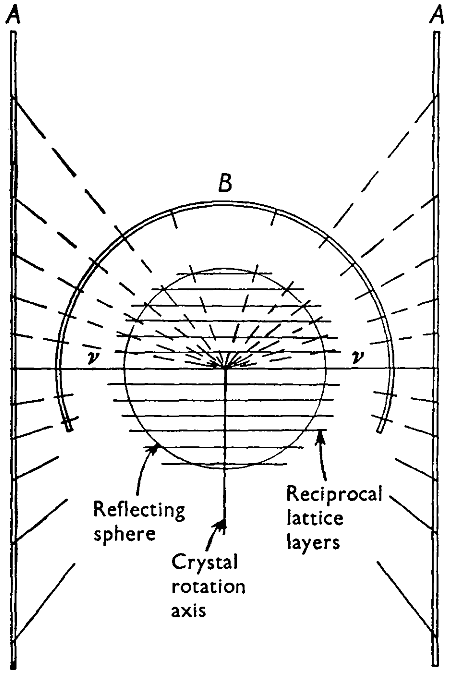

Fig. 1. Rotating-crystal technique with film in the standard position $A$ and in the modified position $B$ permitting normal incidence of reflexions. The direct X-ray beam is normal to the plane of the paper and the diagram illustrates the section at $2\theta = 90°$.

$\cot \nu$ term in (2), since the modified mounting would record the region lost by the conventional film mounting. Thus, in Fig. 1, for the identity period illustrated, the normal mounting $A$ would record only five layer lines, whereas the modified mounting $B$ would record six (see data for ($\pm$)-*iso*cryptopleurine methiodide in Table 1).

From (1) and (2), it is evident that the values of the identity period calculated from the layer lines approach the true value at $\nu = 90°$. This suggestion regarding *identity periods* parallels that by Kettmann for *spacings* (Buerger, 1942, p. 409). To permit satisfactory extrapolation to be carried out, some knowledge of the form of the curve is necessary. A full treatment of all sources of error is not considered suitable or necessary at the present juncture, but the effect of the error arising from eccentricity, the most likely source of error, has been calculated (see Appendix). It has been shown that, in this case,

$$\frac{\Delta a}{a} = K_1\left(1-\frac{2}{\pi}\cdot\frac{\frac{1}{2}\pi-\nu}{\cos\nu}\right)\cos^2\nu\,.\,\mathrm{cosec}\,\nu\,.$$

Therefore the plot of the calculated values of identity periods against

$$\left(1-\frac{2}{\pi}\cdot\frac{\frac{1}{2}\pi-\nu}{\cos\nu}\right)\cos^2\nu\,.\,\mathrm{cosec}\,\nu$$

should permit a straight-line extrapolation to the most accurate value. Omission of the less accurate low-$\nu$ terms would permit extrapolation to be carried out on the plot against the simpler function $\cos^2\nu\,.\,\mathrm{cosec}\,\nu$ (see Appendix).

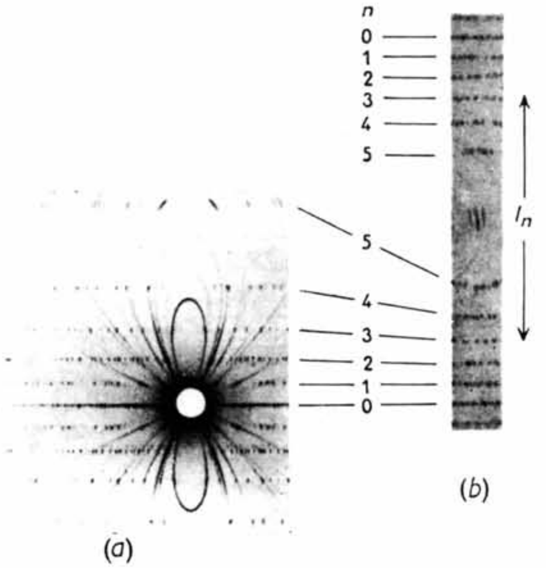

Fig. 2. Comparison for the same crystal of rotation films in (*a*) the conventional film mounting and (*b*) the modified mounting. The layer lines are indicated. In (*b*) $l_n$ is the distance between the $n$th layer lines at $2\theta = 90°$; $l_0 = \pi r$. The crystal is ($\pm$)-pyroglutamic acid.

## Experimental

Herzog & McLachlan (1954) have used a specially prepared spherical photographic surface to demonstrate the complete diffraction pattern from a rotating crystal, but their experimental arrangement is not practicable for general use. We have used instead a half-inch strip of film bent into a hemi-cylindrical shape with the film-cylinder axis coincident with the X-ray beam and positioned to record reflexions in the region $2\theta = 90°$ (Fig. 1 (position $B$)), so that the strongest reflexions are of the same order of intensity over the whole film and the spot size is reasonably constant. Fig. 2 compares a conventional rotation film with the corresponding film in the modified mounting. $l_n$ is the distance on the film (Fig. 2(*b*)) separating the intercepts of the $n$th layer at $2\theta = 90°$ (see Figs. 1 and 5). Intersection of the two portions of the zero layer with the film provides an internal record of the film radius, permitting the angles $\nu_n$ to be measured directly (Table 1).

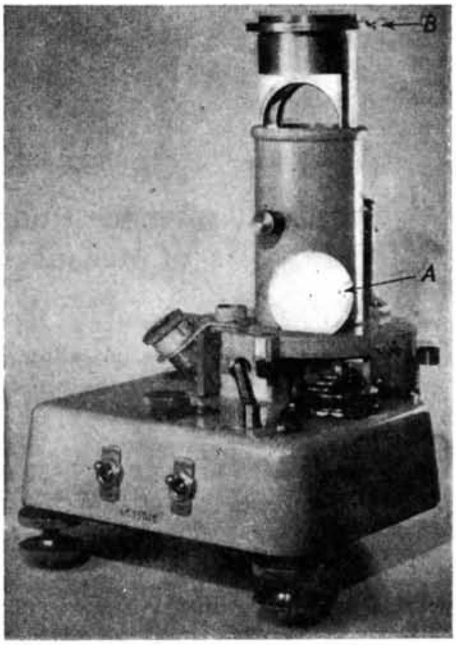

Fig. 3. The adapter displaced from its position in the rotation camera to show some details of construction.

To obtain such films easily and conveniently, a simple film-holder has been designed, Fig. 3, which can be slid into position in the standard film holder of the rotation camera and then held in position by a lock-screw. The film is held in position against a cylindrical surface of radius 2·68 cm. by narrow phosphor-bronze springs. Centring adjustment is obtained by the use of the centring disc, $A$, which makes a sliding fit into the film-holder proper. Vertical adjustment to permit alignment of the centring disc with the X-ray beam is achieved by the screw collar, $B$, at

Table 1. *Measurement of identity period with the adapter*

$\lambda(\text{Cu } K\alpha) = 1{\cdot}542$ Å

| $n$ | (*a*) (±)-Pyroglutamic acid | | | (*b*) (±)-*iso*Cryptopleurine methiodide | | | (*c*) (±)-*iso*Cryptopleurine methiodide | | |
|---|---|---|---|---|---|---|---|---|---|
| | $l_n$ (cm.) | $\frac{1}{2}\pi-\nu_n$ (°) | $a$ (Å) | $l_n$ (cm.) | $\frac{1}{2}\pi-\nu_n$ (°) | $a$ (Å) | $l_n$ (cm.) | $\frac{1}{2}\pi-\nu_n$ (°) | $a$ (Å) |
| 0 | 8·43 | 90·00 | — | 8·42 | 90·00 | — | 7·96 | 90·00 | — |
| 1 | 7·52 | 80·28 | 9·134 | 7·60 | 81·24 | 10·117 | 7·15 | 80·85 | 9·697 |
| 2 | 6·60 | 70·46 | 9·222 | 6·75 | 72·16 | 10·067 | 6·29 | 71·12 | 9·529 |
| 3 | 5·62 | 60·00 | 9·251 | 5·85 | 62·54 | 10·023 | 5·44 | 61·51 | 9·699 |
| 4 | 4·50 | 48·04 | 9·223 | 4·88 | 52·17 | 10·055 | 4·48 | 50·66 | 9·731 |
| 5 | 3·10 | 33·10 | 9·203 | 3·72 | 39·77 | 10·020 | 3·42 | 38·67 | 9·873 |
| 6 | — | — | — | 2·09 | 22·34 | 10·001 | 1·90 | 21·48 | 9·941 |
| Extrapolated value in Fig. 4 | | | $9{\cdot}18_5$ | | | $9{\cdot}99_0$ | | | |

$(\frac{1}{2}\pi-\nu_n)^\circ = (l_n/l_o)\times 90^\circ$

the top of the adapter. Once adjusted, it is fixed by a lock-screw.

Results obtained with this adapter for two crystals, (±)-pyroglutamic acid and (±)-*iso*cryptopleurine methiodide (Fridrichsons & Mathieson, 1955) are recorded in Table 1, in which (*a*) and (*b*) refer to data obtained with the adapter approximately correctly set while (*c*) refers to data obtained with the adapter deliberately and grossly mis-set, the crystal being 2·3 mm. vertically above the centre of curvature of the film. In Fig. 4, identity periods calculated from equation (1) for the various layers are plotted against

$$\left(1-\frac{2}{\pi}\cdot\frac{\frac{1}{2}\pi-\nu}{\cos\nu}\right)\cos^2\nu\,.\operatorname{cosec}\nu\,,$$

the probable spread of each value being obtained from equation (2) by assuming a possible error of 0·1 mm. in the measurement of $l_n$ so that $\Delta\nu=\pm\Delta l/r=\pm 1/268$. Extrapolation of data (*a*) and (*b*) for the approximately correctly-set crystals leads to values of 9·19 Å ($9{\cdot}18_5$ Å) for (±)-pyroglutamic acid and 9·99 Å for (±)-*iso*cryptopleurine methiodide. The identity periods measured from the various layer lines of the crystal misplaced 2·3 mm. are compared in Fig. 4(*c*) with the theoretical values calculated from equation (3) (Appendix) by substituting $p = 2{\cdot}3$ mm. and $r_0 = 26{\cdot}8$ mm. It is clear that, even with this gross mis-setting, extrapolation yields a value within 0·01 Å of the correct value.

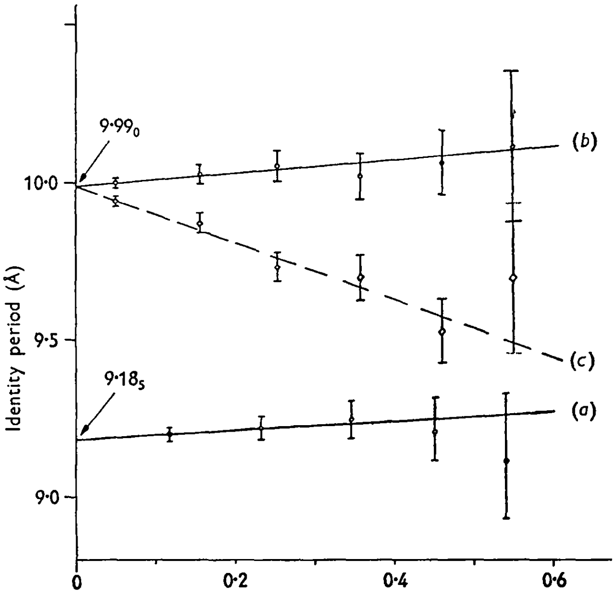

Fig. 4. Values of identity period plotted against

$$\left(1-\frac{2}{\pi}\cdot\frac{\frac{1}{2}\pi-\nu}{\cos\nu}\right)\cos^2\nu\,.\operatorname{cosec}\nu\,.$$

(*a*), (*b*) and (*c*) as in Table 1. For (*a*) and (*b*), the straight-line extrapolations are shown. For (*c*), the dashed line refers to the theoretical distribution of $a' = a-\Delta a$ calculated from equation (3) (Appendix).

Hence, it would appear that extrapolation of the data to $\nu = 90°$ tends to eliminate systematic errors and permits an accuracy of the order of 0·1% in the measurement of identity periods, whereas conventional rotation photographs are generally quoted as accurate to about 0·5–1·0%. This increase in accuracy is achieved without modification of the available equipment. The simple adapter is limited in accuracy since it is essentially a normal-beam unit operating in the $2\theta = 90°$ region. Greater accuracy could be achieved in the measurement of identity periods by operating in the equi-inclination mode to record layer lines in a region close to $2\theta = 180°$. However, this would involve considerable modification to the standard crystal goniometer.

My thanks are due to Mr A. F. Beecham of this Section for providing crystals of (±)-pyroglutamic acid.

## APPENDIX

If the crystal $X$ is displaced a distance $p$ along the rotation axis from the centre of curvature $C$ of a film of radius $r_0$ (Fig. 5), then

$$r = r_0-p\cos\mu,\quad\text{where}\quad \mu = \tfrac{1}{2}\pi-\nu\,.$$

The separation of intercepts of any layer line is given by

$$l = \int_{-\mu}^{+\mu}(r_0-p\cos\mu)d\mu = 2r_0\mu-2p\sin\mu\,.$$

For the zero layer we have

$$\mu = \tfrac{1}{2}\pi, \quad \text{so that} \quad l_0 = \pi r_0 - 2p\,.$$

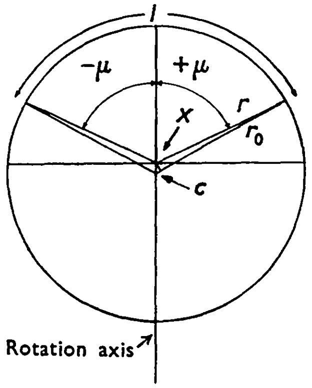

Fig. 5.

The measured value of $\mu$ is $\mu' = \tfrac{1}{2}\pi(l/l_0)$ (see Table 1), so that

$$\Delta\mu = \mu - \mu' = \frac{\pi p}{\pi r_0 - 2p}\left(\sin\mu - \frac{2}{\pi}\cdot\mu\right).$$

We note that $\Delta\mu \to 0$ as $\mu \to 0$. Substituting for $\mu$ and $\Delta\mu$ in equation (2), we have

$$\frac{\Delta a}{a} = \frac{\pi p}{\pi r_0 - 2p}\left(1 - \frac{2}{\pi}\cdot\frac{\frac{1}{2}\pi - \nu}{\cos\nu}\right)\cos^2\nu\,.\,\mathrm{cosec}\,\nu\,. \qquad (3)$$

In the region of extrapolation, where $\mu \to 0$, the quantity in brackets does not vary very rapidly, so we may justifiably write

$$\frac{\Delta a}{a} = K\cos^2\nu\,.\,\mathrm{cosec}\,\nu\,.$$

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*Acta Cryst.* (1957). **10**, 354

# Fourier Transforms in Cylindrical Co-ordinates

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(*Received* 26 *November* 1956)

A brief account is given of some of the mathematics pertinent to the calculation of Fourier transforms in cylindrical co-ordinates, and a systematic derivation is given of the Fourier transforms of a number of curves and surfaces which are most naturally expressed in cylindrical co-ordinates.

## 1. Introduction

Recent interest in the helical structures found in certain molecules of biological origin has drawn attention to the need for studying Fourier transforms in cylindrical co-ordinates. The transforms which have been used have been worked out by a variety of different techniques, and the purpose of this note is to collect together and give a systematic derivation of the transforms of a number of configurations most naturally expressed in cylindrical co-ordinates. Some of the relevant mathematics is briefly discussed, and attention is drawn to the $\delta$-function for the description of curves and surfaces in space. The $\delta$-functions used have been properly normalized in terms of the line- and surface-densities of the diffracting material.

## 2. The $\delta$-function and its applications

The $\delta$-function introduced by Dirac (1930) is not strictly a function at all, although it has gained mathematical respectability since the work of Schwartz (1950), and the way in which it is used may be regarded as a quick method of obtaining results which should then be verified by more exact analysis; but in physics this verification is seldom necessary.

The following properties of the $\delta$-function will be used:

$$\delta(x) = \int_{-\infty}^{+\infty} \exp\,[2\pi i x t]\,dt\,, \qquad (1)$$

$$\delta(x) = \lim_{\alpha\to\infty} \frac{\sin\,(2\pi\alpha x)}{\pi x}\,, \qquad (2)$$

$$\int_{-\infty}^{+\infty} f(x)\delta(x-a)\,dx = f(a)\,. \qquad (3)$$

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