from exposure to the atmosphere, as even brief contact with water vapor caused immediate deterioration. Protection was effected by coating the crystals with a very thin layer of cellulose nitrate obtained by dipping the crystal in a 4% neutral amyl acetate solution before mounting. In this way it was possible to preserve the crystals for several days.

Weissenberg photographs were taken of the equator and first and second layer lines with the crystal rotated about the *c* axis, which was parallel to the long dimension of the crystal. These photographs were obtained through facilities made available by Prof. B. E. Warren of the Massachusetts Institute of Technology. In this laboratory, additional rotation photographs were taken of the crystal rotated about the *a* and *b* axes. It was observed that the *a* and *b* axes lie in directions approximately 45° to the crystal faces. The unit cell was found to be orthorhombic with the following dimensions:

$$a = 11{\cdot}64, \quad b = 9{\cdot}05, \quad c = 5{\cdot}18\ \text{A}.$$

The following systematic absences were observed: $h00$ with h odd, $0k0$ with k odd and $00l$ with l odd. These indicate that the space group is $P2_12_12_1$. The density of the proline crystals, as determined by flotation in a mixture of *p*-bromotoluene and *n*-butyl bromide, was 1·35 g.cm.$^{-3}$. The number of molecules per unit cell was calculated to be 3·9. This indicates that the unit cell contains four molecules.

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A photoelectric device for the evaluation of structure factors.

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Introduction

One of the most important needs in structure analysis is a means for the rapid assessment of the correctness or otherwise of a proposed structure. The device described in this note is a first step towards filling this need, and we hope to develop it into a much more versatile instrument.

Theory

Huggins (1945) has described the preparation of masks (for use in photographic Fourier synthesis) in which the transmission of light at any point is proportional to $1 \pm \cos 2\pi(hx+ky)$, the symbols having the usual meanings. If an image of one of these masks, with positive sign, is projected on a template in which small holes have been drilled with centres at (x, y), the light transmitted will be proportional to $\Sigma A\{1+\cos 2\pi(hx+ky)\}$, where A is the area of each hole. Thus, if the holes are made to correspond in position to the atoms in a proposed structure, with areas proportional to their scattering factors, the value of the summation is proportional to $F(000)+F(hk0)$.

Experimental test

By means of a film-strip projector, modified to give unit magnification, images of the Huggins' masks were projected on a brass template in which holes of about 1 mm. diameter were drilled to represent the structure of durene (Robertson, 1933) projected on to (010). A barrier-layer photocell was placed immediately behind the template and was connected to a galvanometer, the sensitivity of which was so adjusted that the zero reading corresponded to $-F(000)$ and the reading with no mask in position corresponded to $+F(000)$; then the readings with the various masks in position should be equal to the corresponding structure factors uncorrected for change in scattering factor. The following table gives the result of this test. It will be noted that, although there are a few large discrepancies in magnitude, all the signs are correctly derived:

hkl	F(calc.)	F (from machine)
000	+148	+148
200	+ 36	+ 24
400	− 24	− 24
600	− 33	− 50
800	− 48	− 22
001	+ 50	+ 35
002	− 65	− 52
003	− 63	− 73
004	− 1	− 7
005	− 5	− 5
201	+ 21	+ 22
$20\bar{1}$	+ 53	+ 37
202	+ 8	+ 30
$20\bar{2}$	− 4	− 9
203	− 25	− 21
$20\bar{3}$	− 62	− 32
204	− 40	− 53
$20\bar{4}$	− 19	− 2
401	+ 3	+ 12
$40\bar{1}$	− 32	− 41
601	− 89	− 63
$60\bar{1}$	+ 12	+ 17

Sources of error

It is rather difficult to align the image of the mask accurately on the template. Moreover, the method assumes that the photocell has a linear response and that the response is uniform over the whole surface.

These sources of error could be eliminated by allowing a magnified image of the masks to fall on a set of photocells representing atoms; the outputs could be fed through potentiometers, set to allow for different scattering factors. With this device different atomic arrangements could be tried more quickly. Moreover, if the outputs were fed to further potentiometers set to correspond to the appropriate values of $\cos 2\pi lz$ or $\sin 2\pi lz$, values of $F(hkl)$ could also be determined in sets with constant l. This would have great utility in three-dimensional work.

References

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