Photography of Crystal Structures

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Citation: The Journal of Chemical Physics **12**, 520 (1944); doi: 10.1063/1.1723902
View online: http://dx.doi.org/10.1063/1.1723902
View Table of Contents: http://scitation.aip.org/content/aip/journal/jcp/12/12?ver=pdfcov
Published by the AIP Publishing

Letters to the Editor

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Photography of Crystal Structures

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November 1, 1944

AS shown by the writer[1] several years ago, Sir Lawrence Bragg's[2] method of photographic summation of Fourier series by addition of the proper patterns of light and dark bands can be improved in accuracy and speed by the use of a previously prepared set of masks.

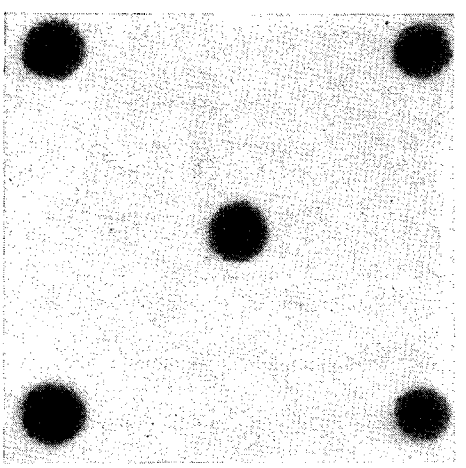

FIG. 1. Photograph, looking along one of the crystallographic axes, of the body-centered cubic unit of α-iron, from x-ray data by Armstrong.

With the assistance of the Physics Department of these Laboratories, an improved set of 316 masks for this purpose has recently been made. Using these, electron density photographs of crystal structures and Patterson summations are easily and rapidly made from the appropriate x-ray data. Examples are shown in Figs. 1–3. The magnification is of the order of 100,000,000 in each case.

Most of the background density, between the atoms, in Fig. 3[3] is not real, but is a result of inaccuracies in the x-ray data and in the masks and incompleteness of the former. The relative positions and approximate relative densities of the atomic peaks are correctly shown, however. In Fig. 1,[4] the background was removed by a short treatment with Farmer's reducer solution. In Fig. 2[5] the background has been practically all removed by reprinting.

The shape of the molecule in Fig. 2 is somewhat distorted, both because the plane of the molecule is not parallel to the plane of the projection and because the projection, as obtained, is a square, whereas the true projection of the unit cell is not. The latter cause of distortion can readily be removed, if desired, by adding another optical step or in other ways. For purposes of structure analysis, however, this is not necessary.

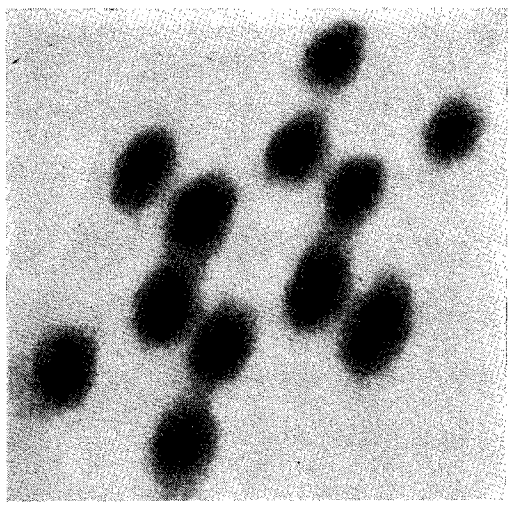

FIG. 2. Photograph of the hexamethylbenzene molecule, using x-ray data from the crystal, by Brockway and Robertson.

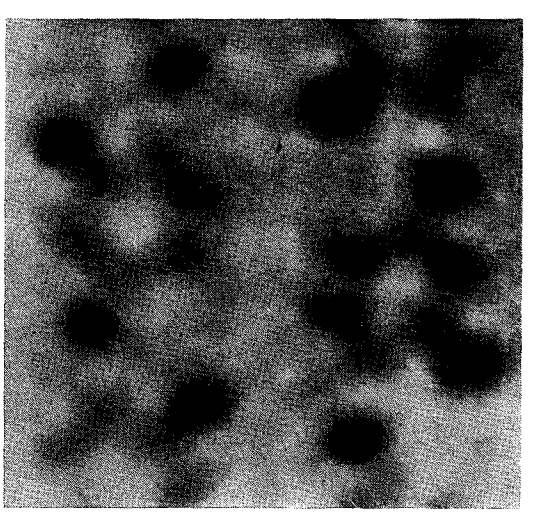

FIG. 3. Photograph of a β-resorcinol (*meta*-dihydroxybenzene) crystal, using x-ray data by Robertson and Ubbelohde. Two complete molecules, with parts of others, are shown.

We hope soon to be able to furnish duplicate copies of the improved set of masks, at a nominal cost, to others engaged in crystal structure analysis.

[1] M. L. Huggins, J. Am. Chem. Soc. **63**, 66 (1941).
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[3] J. M. Robertson and A. R. Ubbelohde, Proc. Roy. Soc. **A167**, 122 (1938).
[4] A. H. Armstrong, Phys. Rev. **34**, 931 (1929).
[5] L. O. Brockway and J. M. Robertson, J. Chem. Soc., p. 1324 (1939).