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A SIMPLIFIED REPRESENTATION OF OPTICAL FOURIER SYNTHESIS

The projection of electron density of a crystal on appropriate plane by inverse Fourier transformation is the mathematical equivalent of image formation by optical instrument. The artificial reproduction of image of crystal structure by optical interference as suggested by Bragg needs a set of coherent monochromatic beams of light, simulating a zone of diffracted X-ray beams in intensity, phase and spatial distribution. This is usually achieved by drilling holes of different sizes in opaque disc and using mica plate in this mask for introducing necessary phase differences. The difficulty of drilling holes of different sizes to take account of the whole zone of reflexions may be circumvented by photographic reproduction of an appropriate weighted reciprocal lattice section. But, lack of uniformity in optical thickness of photographic plate offsets the task of preparation of diffraction mask of appropriate size to be used advantageously in Optical Diffractometer with fairly large lens.

We have seen that a very much simplified procedure for preparing a mask can be adopted in suitable cases and yet a fairly satisfactory image can be obtained using Optical Diffractometer with 4\(^\circ\) lens system. The (hol) projection of platinum phthalocyanine is centrosymmetrical and satisfied the condition that phases of all the reflexions are positive. The structure factors of hol zone of reflexions are divided into four groups roughly in order of their magnitude so that the average value of F's of these groups are approximately proportional to (1.5\(^2\)), (1\(^2\)), (0.75\(^2\)) and (0.5\(^2\)). A reciprocal lattice net is drawn using a scale of 20 cm to 1A\(^0\)-1. A mask is prepared on reduced scale (using a pantograph punch) of reduction ratio 12:1 on a strip of exposed film, punching holes of diameter 1.5 mm, 1 mm, 0.75 mm and 0.5 mm, a particular size of hole being used to represent an entire group of reflexions. The areas of the holes representing a group are thus made roughly proportional to average F values of the corresponding group. The size of the hole representing F (000) has been chosen arbitrarily. The image of the platinum phthalocyanine molecule obtained as the diffraction pattern of this mask is shown in Fig. 1a with a trace of the molecular feature superimposed upon it. The mask is shown alongside. The calculated electron density map is shown in Fig. 1b for comparison.

A few spurious peaks that are observed in the diffraction pattern might well be accounted for the gross representation of the Fourier components. Due to series termination effect diffraction ripples can be noticed in the calculated electron density map as well. Though no accuracy could be claimed by such an approach, its usefulness in structural investigation, particularly in quick optical representation of approximate Patterson function is worthy of exploration.

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