

International Union of Crystallography Congress in Rome, 9–14 September 1964

Automatic Single-Crystal Diffractometry for X-rays and Neutrons

During the Sixth Congress of the International Union of Crystallography in Rome, September 1963, the Commission on Crystallographic Apparatus held two Open Sessions on 'Automatic Single-Crystal Diffractometers for X-rays and Neutrons'. Three invited lectures were devoted to the X-ray and three to the neutron technique. Not all texts are available but, for the four which follow, the authors have been kind enough to permit presentation as a group. In this form they provide a valuable assessment

of the contemporary state of development in single-crystal diffractometry. They have been prepared for publication by the Chairman of the Commission on Crystallographic Apparatus (Dr A. McL. Mathieson), and the Editors of *Acta Crystallographica* are grateful for his help. Abstracts of the two papers for which the full text is not available will be found on p. A 152 of Volume 16 of *Acta Crystallographica*.

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Analogue and Digital Single-Crystal Diffractometers

BY U. W. ARNDT

Medical Research Council, Laboratory of Molecular Biology, Hills Road, Cambridge, England

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Automatic diffractometers which have been described to date fall into one of three classes: those in which an automatic systematic search is made for the Bragg reflexions, those in which the angular positions of the crystal and detector axes are computed by means of an analogue computer which is generally an integral part of the diffractometer, and those in which these positions are computed by a digital computer. The first two types of instrument are commonly referred to as analogue diffractometers while diffractometers of the third type are called digital. In this last type the computer may or may not be directly linked to the diffractometer control circuits; in either case digital shaft positioning methods are used, similar to those employed in automatic machine tool control. Within all three classes of diffractometer a variety of different geometrical arrangements is possible.

The actual measurement of a reflexion in all these instruments requires the determination of the integrated intensity and of the background level near the Bragg peak. Stationary or moving crystal methods may be used.

The relative merits of automatic diffractometers must be assessed according to a variety of different considerations.

Introduction

The types of problem investigated by means of X-ray diffraction studies on single crystals cover a wide range. They include such widely divergent subjects as, on the one hand, very accurate electron density determinations on small molecules whose structures are already known to a high degree of approximation, and on the other hand the determination of the structures of very large completely unknown biological molecules; they cover high and low temperature studies, the investigation of thermal diffuse scattering, molecular weight determinations and investigations of crystal imperfections. For the thirty years or so during which the vast majority of crystallographic studies were carried out almost exclusively by photographic methods, a large number of special X-ray cameras were evolved and many different techniques were devised.

Developments in the reliability and sensitivity of X-ray detectors and associated circuitry, in techniques of automation and in the processing of experimental data by means of digital computers have stimulated the desire to replace X-ray cameras and densitometers by automatic diffractometers using quantum counters as detectors. There has been much mutually beneficial interplay between such developments in X-ray diffraction and in neutron diffraction where photographic techniques are more difficult and where these were developed relatively late in the growth of the subject.

As there is no universal photographic technique which will suit all crystallographic problems so there can be no one type of automatic diffractometer which is 'best' for all purposes. It should, perhaps, be said here that while much valuable work has been done, and continues to be done with non-automatic X-ray diffractometers, manually operated instruments repre-