# INTERNATIONAL TABLES

# FOR

# X-RAY CRYSTALLOGRAPHY

VOL. I. SYMMETRY GROUPS

VOL. II. MATHEMATICAL TABLES

VOL. III. PHYSICAL AND CHEMICAL TABLES

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**Volume II. ERRATA**

**p. 46.** Last sentence: for *the last two cases* read *cases* (*c*) *and* (*d*).

**p. 186.** The diagram is inverted. Correction needed in the legend: for *bottom* read *top*.

# CONTENTS

**5.2. Intensity of Radiation Diffracted by a Crystal** (*continued*) PAGE

# 1. INTRODUCTION

JOHN KASPER

## 1.1. Purpose and Scope of the Tables

The present Volume contains information primarily of a mathematical nature and is characterized by the absence of physical data, which are compiled in Volume III. It comprises tables of functions, formulae and geometrical diagrams that for the most part are strictly mathematical, even though they may pertain to the application of a physical effect (for example, a table of $\exp[-B(\sin\theta/\lambda)^2]$ is given for applying the effect of temperature motion on diffracted intensities). There are included, as well, general relationships between physical quantities, but essentially none of the material is of a kind to require revision on the basis of improved physical measurements.

It is intended that this Volume should be useful in many stages of a crystal-structure determination: in the recording of X-ray diffraction effects; in the indexing of the recorded diffraction data; in the correction of intensities for geometrical and physical factors; in the production of vector and electron-density maps; and in the calculation of structure factors. Appropriate material is provided also for various other aspects of crystallographic research and the utilization of X-ray diffraction effects. A special feature is the inclusion of a comprehensive compilation of basic mathematics. This should serve a dual purpose: a utilitarian one is that of providing those simple items of mathematics which may occur in standard handbooks and texts but to which the crystallographer needs to make frequent reference; a second aim is to make available in a uniform treatment those mathematical topics that are basic to theoretical structure work but which occur in a scattered way, often with different notations, in a very extensive literature.

## 1.2. Arrangement of Tables

The decision on the division of the contents into the various sections and on the placement of the tabular material has been made on the basis of affording maximum convenience in the use of the Volume. In practice, at a given stage of a structure investigation one usually needs to consult only the material of one of the sections. The section headings themselves suggest the nature of their contents and the aspect of structure work to which they are applicable.

It seemed natural to have the basic mathematics (Section 2) precede all other material. Crystal geometry (Section 3) contains subject matter conventionally associated with the title. It includes the quadratic forms which are required for deducing interplanar spacings and for indexing powder patterns. The section has been subdivided according to crystal system, since generally one will wish to consult it in regard to one particular crystal or substance. Sections 4 and 5 have to do with diffraction methods and effects; Section 4 is principally concerned with the recording of data; Section 5 with the various factors modifying the intensity of a diffracted beam. The special role of Fourier methods in crystal-structure problems makes desirable a separate Section 6 devoted to them. Three special topics are classified separately in Section 7. Finally, the extensiveness of the tables of $\sin 2\pi hx$ and $\cos 2\pi hx$ has made it seem worth while to include them along with other trigonometric and exponential tables separately as Section 8, in the convenient location of the final pages of the book.

The accuracy and reliability of the various tables is discussed in the appropriate sections.

Some charts are given for illustrative purposes. In keeping with the general policy of the Editorial Commission, no attempt has been made to make them suitable for direct use. Tables are given for the construction of charts. Many such charts may now be purchased, and information about those currently available can be obtained through some National Committees or Associations. A separate card gives a Table of Proportional Parts.

## 1.3. Acknowledgments, etc.

The General Editor acknowledges indebtedness to the various authors who have contributed to this Volume, and to proof-readers. Many others have helped in ways too varied to enumerate; some, but not all, have received mention at various stages in the Volume. The staff of The Kynoch Press have taken the greatest possible trouble to see that this volume is as well produced as was Volume I and are in no way responsible for the time that has elapsed between the publication of the two volumes.

In general, notification of numerical or other errors should be made to the General Editor, although in case of doubt direct contact with the author concerned may be more helpful.

# Section 2

# FUNDAMENTAL MATHEMATICS

A. L. PATTERSON