Preface

International Tables for Crystallography started life in in 1935 as a two-volume set entitled *Internationale Tabellen zur Bestimmung von Kristallstrukturen*, with C. Hermann as editor. We are now in the third series, with eight volumes covering all aspects of crystallography from symmetry to macromolecular crystallography. However, there has always been one glaring omission and one that has become increasingly serious: powder diffraction. This is odd: powder crystallography started as early as 1916 with the seminal work of Debye and Scherrer, and has grown to include quantitative and semi-quantitative analysis, structure solution and refinement, two-dimensional data, comprehensive databases, clustering, and microstructural properties, and is applied to a wide range of problems of both academic and industrial interest. Articles in the International Union of Crystallography's monthly *Journal of Applied Crystallography* are dominated by powder-diffraction papers. In terms of instrumentation, there are more powder diffractometers (∼10 000) in use worldwide than any other comparable diffraction instrument. There have also been rapid advances in radiation sources and detectors, and major developments in software, computing power and visualization tools, all of which have made what was once cutting-edge science commonplace.

The methodology that has done more than anything to transform the field treats the measured powder-diffraction data in a comparable way to single-crystal data (albeit with more restrictive conditions) and is generally known as Rietveld refinement. This method will be found everywhere in this volume and was developed in the 1960s by Bert Loopstra (who came up with the concept), Bob van Laar (who worked out the mathematics) and Hugo Rietveld (who wrote the first computer program for it), as discussed in a recent article by van Laar & Schenk [*Acta Cryst.* (2018), A**74**, 88–92].

The field has not been devoid of books: there are excellent books edited by Dinnebier and Billinge [*Powder Diffraction Theory and Practice* (2008), Cambridge: Royal Society of Chemistry], Clearfield, Reibenspies and Bhuvanesh [*Principles and Applications of Powder Diffraction* (2008), Oxford: Wiley] and Mittemeijer and Welzel [*Modern Diffraction Methods* (2013), Weinheim: Wiley-VCH]. These, however, are not completely comprehensive and the need for a volume of *International Tables* dedicated to powder diffraction has become increasingly urgent.

So here it is. As if to emphasize the scale and diversity of the topic, it is one of the larger volumes of *International Tables* with over 900 pages and 54 chapters. The first part is devoted to basic diffraction theory as applied to powder samples, followed by parts on instrumentation and sample preparation, methodology, structure determination, defects, texture and microstructure, and software, and concluding with descriptions of applications over a wide variety of disciplines ranging from ceramics to pharmaceuticals. Even a volume of this size cannot be wholly comprehensive, but the editors hope that it covers a wide range of topics that will be relevant and of interest to most powder diffractionists. We plan to include yet more topics in a second edition.

The volume is intended primarily to be a practical one – when you have a problem in powder analysis this should be the first book you reach for. To this end, the data for many of the examples discussed in the text can be downloaded from https://it.iucr.org, so that readers can try the examples for themselves. We have not (yet) included step-by-step instructions on how to process the data; perhaps that will come in the future. The chapter on software gives information on how to obtain the necessary programs.

A word is needed about notation. A field as diverse as powder diffraction does not have a uniform notation. Texture and stress, for example, use a different nomenclature to structure solution. Our conclusion was that if we were to attempt to impose a uniform notation throughout the volume, it would have made it very difficult to link the chapters to the existing literature. We have to live with diversity.

An enterprise such as this has been a large undertaking, and we thank the authors for their patience. It is important to acknowledge the role of the staff at the IUCr offices in Chester, especially Nicola Ashcroft, Simon Glynn and Peter Strickland. We are very grateful for all their hard work.

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Editors, *International Tables for Crystallography* Volume H