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## **Preface**

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In May 2010, during a meeting of the International Programme Committee for the Twenty-Second Congress and General Assembly of the International Union of Crystallography (IUCr), discussions started between C. J. Gilmore and Isabella Ascone (then Chair of the IUCr's Commission on XAFS) about the possibility of including XAFS-related information in a new volume of *International Tables for Crystallography* that would cover mainly powder-diffraction techniques. After the IUCr decided to dedicate one volume to powder diffraction (subsequently published in 2019 as Volume H of the series) and a separate one to the XAFS technique, the Commission on XAFS submitted a detailed document with suggestions for the content of this Volume I to the IUCr Editorial Office at the beginning of December 2010.

This first proposal was composed primarily by I. Ascone with assistance from C. T. Chantler (then Secretary of the Commission). As Chair of the Commission, I. Ascone started many challenging projects, including looking at XAFS data formats, the standardization of XAFS experimental procedures, contributing XAFS-related definitions to the IUCr's Online Dictionary of Crystallography at https://dictionary.iucr.org ('the XAFS dictionary'), work towards this volume of *International Tables*, and fostering close cooperation with other IUCr commissions and with the International XAFS Society (IXAS) at IUCr Congresses and in the organization of workshops. These projects progressed well as the XAFS Commission was a highly functioning team. The dataformat work led to the inauguration of a series of Q2XAFS (Quality and Quantity in XAFS Spectroscopy) conferences as a joint project with IXAS, then led by Hiroyuki Oyanagi, resulting in many publications in IUCr journals as an outcome of the meetings.

Great support for the *International Tables* project was provided by the IUCr Executive Committee, including Sine Larsen and M. L. Hackert; Michael Dacombe; Samar Hasnain; and indeed the Chair of the Commission on *International Tables*, Carol Brock. From early on, it was planned that, as far as possible, different experimental and theoretical backgrounds and regional approaches should be presented, in particular to bring the whole international XAFS community together to share their amassed knowledge. In 2013, three editors for the volume were appointed: Professor Christopher Chantler (Australia), Professor Bruce Bunker (USA) and Professor Federico Boscherini (Italy). The final version of the proposal for the volume was approved by the IUCr's Executive Committee in 2014. The first submissions started to arrive in 2015 and were subsequently fully reviewed and revised before acceptance.

Many chemists, bioscientists and crystallographers often need the supporting evidence and investigations afforded by XAS and XES. Our deliberate purpose is that this volume should be self-contained and, as far as possible with any developing live technique, we intend it to be complete. It has been written for the worldwide XAS community of thousands of practitioners, user communities, beamline scientists, experts and academics, and for the neophyte user who wishes to know what XAS and XES can do for them and how they may use these techniques for their particular purposes. The volume is therefore intended to be an authoritative resource that can be used for training, learning or teaching, providing practical guidance for readers of all levels of experience. It also provides full discussions of the many questions and practical issues that can arise at all stages of XAS or XES experiments and data processing. In addition, it can simply be used as a reference work like a normal *Handbuch* or encyclopaedia, and dipped into for insightful discussion of or solutions to problems or questions.

## international tables

There are smaller-scale works, including textbooks and books, that have provided much insight into XAS and XES, but there is certainly a need for an authoritative and more comprehensive summary such as the present volume. Several authors of these valuable smaller or focused works are also authors of chapters in this volume, which has thus benefitted from their expertise.

The Editors would like to express particular thanks:

To all the expert authors and referees who have contributed outstandingly to so much of this work, and in some cases have not lived to see the fruition of their extensive efforts.

To our fellow Editors, without whom this would not have been possible. We have worked collaboratively and collegially on all aspects of the project. To the team at the IUCr's Editorial Office (Simon Glynn, Nicola Ashcroft and Peter Strickland) for their many hours, months and years of work. We are amazed at their continued energy, enthusiasm and the level of care they have shown for the project.

To Isabella Ascone, whose drive and initiative inspired the Commission, IXAS and the push towards producing this volume.

To Ted Maslen, who guided many of us within and outside crystallography towards the path of accuracy and insight in science.

To the close and warm relations between crystallography, X-ray spectroscopy and all techniques, that we may understand one another better!