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John R. Helliwell

Certifying Central Facility Beamlines for Biological and Chemical Crystallography and Allied Methods



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John R. Helliwell

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John R. Helliwell
Department of Chemistry
University of Manchester
Manchester, UK

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Preface

My aims in writing this Springer Brief book are:—

Firstly, to guide beamline providers and users on what to look for in selecting experiments for a given type of facility and beamline so that beamtime usage and effectiveness are maximised. Secondly, to help them to navigate facility publication, as well as data management and sharing policies, and avoid potential pitfalls between facility and user on these important post experiment aspects. Thirdly I provide tabulations of these experimental facilities globally. Often in my text I express my personal perspectives from my career these past 50 years. That said I am very grateful to the six colleagues who gave me their expert comments, who I list below.

I need to air what is a Springer Brief book? These are defined to be ‘succinct summaries of cutting-edge research and practical applications covering a range of content from professional to academic and featuring compact volumes from between 50 to 125 pages’. The aims (<https://www.springer.com/series/16236>) include such as provide a ‘bridge between new research results and a contextual literature review’ and, rather more challenging, ‘A presentation of core concepts that students must understand in order to make independent contributions’. In general, the word ‘brief’ I think has several different meanings, namely: short duration, concise summary or inform someone thoroughly especially in preparation for a task. The first of these meanings relates to these books being relatively quick to read and hopefully digest. The second meaning is that they are not verbose and are a summary. The third is the more challenging aspect especially so with respect to students where practical experimental experience is as important, or more so actually, as reading a book or having tutorials.

Some 30 years ago I published my *Macromolecular Crystallography with Synchrotron Radiation* research monograph (Helliwell (1992)) which comprised more than 600 pages. At the time I was also heavily involved proposing, developing, and managing beamlines for macromolecular crystallography at the UK’s SRS. My efforts included generating spin off applications into synchrotron radiation chemical crystallography and solution X-ray scattering. I helped launch analytical services to industry, which became the Daresbury Analytical Research Technical Services (known simply as DARTS). The beamlines operating at the UK’s SRS

provided a platform for the proposals for macromolecular crystallography at the European Synchrotron Radiation Project, based at that time in the mid-1980s at CERN in Geneva. These proposals formed a part of the ESRF Foundation Phase Report (1987), which led to the construction of the ESRF as a facility in Grenoble in the 1990s.

My monograph book was published in paperback in 2005. I considered a second edition, but the field had expanded so enormously and had helped to stimulate neutron Laue macromolecular crystallography at the Institut Laue Langevin also in Grenoble, which needed a description alongside the synchrotron applications. Overall, when the opportunity came up to write a Springer Brief book in 2023, I thought ‘aha’ this is a good opportunity to bring the very practical aspects of using beamlines up to date. I hope this Brief book will be as useful as my synchrotron radiation monograph has obviously been, having made it into paperback.

In this Brief Book I have added electron diffraction and electron bioimaging as these are now also operated by the synchrotron radiation facilities. To form as complete a description of the landscape of methods, I have included solution scattering and several spectroscopic methods.

Manchester, UK
October 2024

John R. Helliwell

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I was greatly encouraged in considering writing this Springer Brief by my giving the opening lecture at the Synchrotron radiation Workshop entitled “*A practical approach to synchrotron experiments*”, which was on day zero of the IUCr Congress in Melbourne Australia held in August 2023. This Workshop was splendidly organised by Dr. Dubravka Sisak-Jung under the auspices of the Swiss Crystallography Association.

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