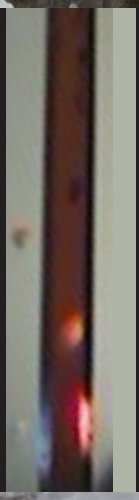
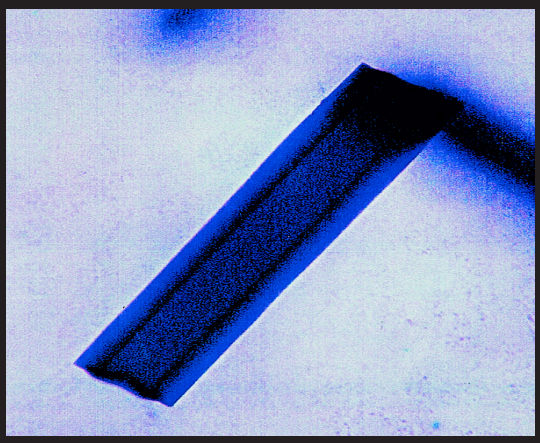
PERSPECTIVES IN CRYSTALLOGRAPHY





John R. Helliwell

CRC Press
Taylor & Francis Group

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CRC Press
Taylor & Francis Group
Boca Raton London New York

CRC Press is an imprint of the
Taylor & Francis Group, an **informa** business

The colourful crystals depicted on the front cover relate to Chapter 6 entitled "The structural chemistry and structural biology of colouration in marine crustacea." They serve as illustrations of the themes of the book including the sustainability of life (Chapter 8). The other crystals are those of 'common salt' (sodium chloride) and relate to the historical aspects of X-ray crystal structure analysis described in Chapters 2 and 3.

The pictures of the crystals shown are with the permission of the publisher International Union of Crystallography, see http://journals.iucr.org/ and of the authors, namely:

Professor Naomi Chayen re Figure 2 from Acta Cryst. (1998). D54, 8-15 doi:10.1107/S0907444997005374 Comparative Studies of Protein Crystallization by Vapour-Diffusion and Microbatch Techniques by N. E. Chayen; the β-crustacyanin (blue) protein was crystallised by Professor Chayen and the protein had been extracted and purified from the European lobster carapace by Dr Peter Zagalsky.

Dr Madeleine Helliwell who grew the various red, and one orange, crystals re the studies of the carotenoids below reported in Acta Cryst. (2007). B63, 328- 337 doi:10.1107/S0108768106052633 Unravelling the chemical basis of the bathochromic shift in the lobster carapace; new crystal structures of unbound astaxanthin, canthaxanthin and zeaxanthin by G. Bartalucci, J. Coppin, S. Fisher, G. Hall, J. R. Helliwell, M. Helliwell and S. Liaaen-Jensen.

CRC Press
Taylor & Francis Group
6000 Broken Sound Parkway NW, Suite 300
Boca Raton, FL 33487-2742

Version Date: 20150917

International Standard Book Number-13: 978-1-4987-3211-6 (eBook - PDF)

To my mother and father; to my wife Madeleine and our son James and daughter Katherine.

In loving memory of Nick Helliwell (1983–2011).

William Blake

(1757–1827)

(From "Auguries of Innocence")

To see a world in a grain of sand
And a Heaven in a wild flower,
Hold infinity in the palm of your hand
And eternity in an hour.

Contents

SECTION IV Societal impacts

Foreword

The International Year of Crystallography was celebrated 2014 by lectures, symposia, articles, new books and web activities. This year was chosen because Max von Laue was the first in the field of crystallography to be awarded the Nobel Prize in Physics 1914 due to his finding in 1912 that a crystal put into an X-ray beam diffracted X-rays. This not only led to the understanding that X-rays are electromagnetic radiation, but the same year William Henry and William Lawrence Bragg realized and showed that the atomic arrangement in crystals could be deduced from the intensities of the diffracted beams. In fact the celebrations of these developments began already in 2012. Among other activities a symposium was held in Adelaide to celebrate the centennial of the groundbreaking experiments by one of the sons of the city, W.L. Bragg. The lectures were published as a special issue of *Acta Crystallographica series A*.

Crystallography has been an extremely fruitful scientific field. In the beginning it gave the first glimpses of an understanding of the atomic organization of simple salts and minerals, but gradually more challenging materials could be analyzed. Not only X-rays were used, but gradually electrons or neutrons added new possibilities to investigate crystal structures. In the 1950s the interest in structures of biological systems led to extremely important steps forward, like the structure of DNA or the first protein structure. These successes have been followed by an extreme flood of structures as complex as ribosomes or whole viruses. Many of the latest developments would not have been possible without the development and usage of synchrotrons, where the radiation initially was a nuisance to the physicists who worked on them but subsequently became an enormous benefit to crystallographers and others who needed intense X-ray beams. The field of crystallography has been instrumental for numerous fields of science where the structural knowledge has led to fundamental new levels of understanding. Therefore this discipline has been awarded at least 20 Nobel Prizes in physics, chemistry and physiology or medicine.

The author of this book, Professor John R. Helliwell, has throughout his scientific career been involved in central activities in the field, not only in determining structures and involved in education, but he has had important roles in the development of experimental possibilities at synchrotrons and also at neutron sources. He has also held central positions like chief editor of the journals published by the International Union of Crystallography as well as being the chair of the European Crystallographic Association. He has written an extensive coverage of how to make best use of synchrotrons for crystallography. The current book contains on one face of it reviews that he has published in *Crystallography Reviews*, a journal for which he is the editor. These articles cover a wide range of topics including historic accounts of crystallography, the evolution and use of synchrotron radiation for crystallography, the possibility of locating the lightest atom, hydrogen, in crystallographic experiments as well as the structural biology behind the coloration of marine crustacea. The book also contains chapters for a more general audience partly focusing on the public understanding of crystallography but also on where the field may be heading and its role in the sustainability of life. It is a book addressing great challenges and is of a broad general interest.

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Preface

The International Year of Crystallography approved by the United Nations and UNESCO took place in 2014. A key message was to build on the achievements of that year. This book aims to contribute to that process. It brings together a wide range of topics to interest both specialists and non-specialists alike. The book opens with a chapter describing my own efforts at explaining crystallography and crystal structure analysis to a wide range of audiences. I then highlight the history of crystal structure analysis. This is followed by several detailed review articles which explain a representative suite of topics in the field of crystallography, concluding this section with a short description of the future of crystal structure analysis in the next 100 years. The book concludes with a chapter describing some of our inputs, as a field, to the sustainability of life.

I am especially grateful to Anders Liljas for agreeing to write the Foreword.

I am very grateful to Hilary Rowe of CRC Press for her wise insights and comments on my book project. I am grateful to the managing editor of *Crystallography Reviews*, Huw Price, for his permission to allow my reviews in *Crystallography Reviews* to be reproduced in this book. I am also grateful to Stu Fisher, Richard Henchman and James Wilkinson for their permission to include our review article as Chapter 5 in this book. I am grateful to Stuart Eyres of Daresbury Laboratory for the 'morph photo' of me onto Dali's picture *Galatea of the Spheres* (see back cover of the book). I first saw this at an exhibition of Dali's art in Rome in a gallery at the Piazza del Popolo. (I was in Rome chairing a workshop on CCD detectors for crystallography held at the Università degli Studi di *Roma* 'La Sapienza' funded by the European community.) Dali (http://en.wikipedia.org/wiki/Galatea_of_the_Spheres), recognising that matter was made up of atoms which did not touch each other, sought to replicate this in his art at the time, with items suspended and not contacting each other. This intertwining of the abstract with the science achieved by Dali in his *Galatea of the Spheres* emphasises, for me, the importance of one's ideas and imagination and the perfecting of one's skills, mathematical and experimental, to progress one's contributions to science.

A short interview with me, briefly describing the International Year of Crystallography, some of my scientific biographical details and my role as editor of *Crystallography Reviews* is available at http://www.chemistryarena.com/06/2014/uncategorized/interview-with-john-helliwell-editor-of-crystallography-reviews.

Overall, I hope that this book of perspectives will be of interest to crystallographers at all stages of their careers from graduate students and post-docs to established academics. In addition, crystallography is enjoying unprecedented public interest arising from the International Year of Crystallography. I also hope then that this book will help sustain the interest of the public and schoolchildren in crystallography.

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Author

John R. Helliwell has wide experience teaching physicists, chemists and biological scientists at undergraduate and postgraduate research levels and ran a research group at the University of Manchester, United Kingdom for over 20 years which has comprised scientists worldwide. Working at the Daresbury Laboratory, up to department head level supervising over 200 staff, greatly broadened his perspectives. In both academic and scientific civil service contexts, he has presented crystallography and research to diverse audiences. He has served the International Union of Crystallography as a representative in several global organisations, including pioneering the general topics of open access of literature linked with crystallographic research raw data. Sustainability of life, mentoring and the importance of gender equality are important elements of his work and efforts. He has chaired science advisory committees in Japan, Australia, the United States and Europe. Professor Helliwell is now emeritus professor in chemistry at the University of Manchester, United Kingdom. He has a DPhil in molecular biophysics from the University of Oxford and a Doctor of Science Physics degree from the University of York. Professor Helliwell is a recipient of the Patterson Award of the American Crystallographic Association and the Perutz Prize of the European Crystallographic Association. He is a fellow of the Institute of Physics, the Royal Society of Chemistry, the Royal Society of Biology and the American Crystallographic Association.