Foreword

As a professional neutron scatterer involved in the business of building, commissioning, operating and increasingly these days, *justifying* the use of instrumentation for single crystal neutron diffraction I feel at least adequately qualified to have written this monograph. To be honest, there are others more qualified and more experienced than I who could have done the job as well or better. But they haven't so here we are.

My aim was originally to cover mostly techniques and in some sense my own "vision" of the future in this area. But it became rapidly apparent to me that to do so would have been to fall into the classic trap of concentrating on the experiment for the experiment's sake, and always to look forward to what might be rather than to appreciate the quality and value of what we are currently doing, and particularly how this is built on the foundations laid by those working in the pioneering days of the late 60s and 70s.

So, the structure of the book has had to evolve. From having one chapter devoted to chemical crystallography and one, shorter, to applications in the biosciences, I found myself confronted with a mass of more than 900 neutron structures of organic materials, and a need to review these comprehensively. This is important both to represent properly the work on which all current and future applications will be based, and to credit appropriately the marvellous and profound work carried out by the pioneers, including Walter Hamilton, Jim Speakman, George Bacon, Mogens Lehmann, Tom Koetzle, George Jeffrey, William Busing, Henri Levy, Carroll Johnson, Phil Coppens, the Uppsala group and many others. So the review chapters have grown into what I hope is a reasonably comprehensive summary of past and present work involving single crystal neutron diffraction applied to molecular systems. I apologise for any misinterpretation or incompleteness but I hope to have kept these to a minimum, and trust that my selection of highlighted topics gives suitable focus to the discussion.

But that is not to underestimate the importance of developments in neutron scattering, sources and instrumentation, for there are pioneers there also: from Nobel laureates Cliff Shull and Bert Brockhouse onwards. The development of instrumentation and data collection methods is therefore also traced and summarised, with particular reference to the increasingly sophisticated applications enabled by these. The nature of neutron scattering also means that sources are a major issue - these are central facilities developed and operated for the common good. The best in reactor and spallation sources are described and the future also mapped out with

particular reference to the new opportunities promised as we attempt to increase the available count rate by factors of five, ten, a hundred or more.

In summary, this book is intended to present a comprehensive account of the techniques and applications of neutron single crystal diffraction in the area of chemical crystallography and molecular structure. I hope to have covered the reasons for choosing to use the technique, the methods both for production of neutrons and their measurement of their scattering by molecular crystals, and given a detailed review of past, present and future applications. Both steady state and pulsed neutron sources and instrumentation are discussed extensively, while the review of applications is, I hope, the most comprehensive yet assembled. The book endeavours to show why the technique is an essential method for studying areas as diverse as hydrogen bonding and weak interactions, organometallics, supramolecular chemistry and crystal engineering, metal hydrides, charge density and pharmaceuticals. My aim has been to provide a reference source for the research worker interested in using neutron diffraction to study the structure of molecules and to reflect some of the exciting and profound achievements in this area.

I therefore hope that this monograph represents a reasonable attempt at summarising past, present and future developments and applications of single crystal neutron diffraction and that it can convey some of the diversity and excitement those of us working in the area feel the technique has to offer.

I thank the ISIS facility for provision of computing facilities and for the working environment which has inspired me in much of my single crystal work. I also thank my colleagues at ISIS and elsewhere who have patiently and kindly enquired about progress on this manuscript, usually as gently as was required. Special thanks are due to Dr Victoria Nield, for her critical readings of the manuscript at various stages.

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November 1999