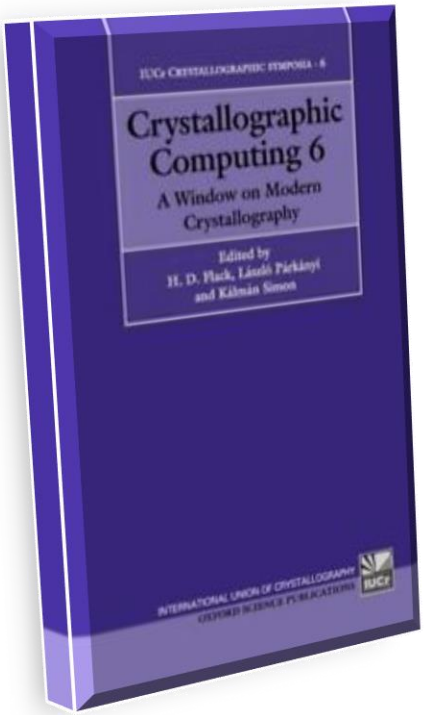


Howard's Web

Brian McMahon

IUCr, Chester, United Kingdom

E-mail: bm@iucr.org

“
Howard had a **brilliant mind** of the **first water**, able to comprehend simultaneously the **finest points of detail** and **the big picture**. He was intrigued by the technical aspects of computer **networking** at the level of protocol and engineering, yet at the same time saw its importance not only in **connecting together** electronic devices, but as a medium for linking concepts, sharing news and information, communicating with colleagues, and ultimately for shaping the community.
”

https://www.iucr.org/people/crystallographers/flack_ep

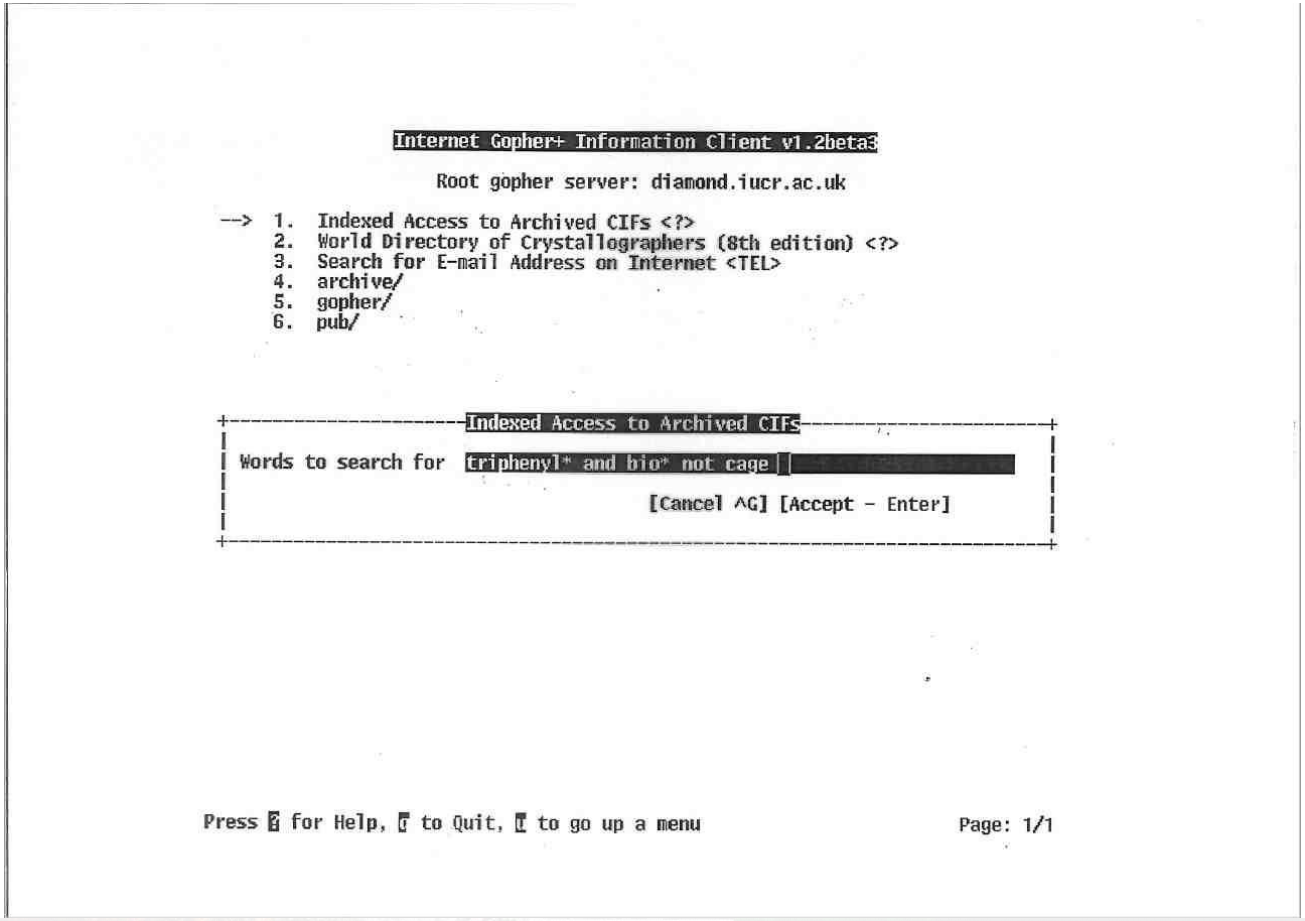
1992: CONCISE – international networking infrastructure

- Distributed information publishing system
- EU funding through RARE (Réseaux Associés pour la Recherche Européenne) for the COSINE (Cooperation for Open Systems Interconnection Networking in Europe) project
- Aimed to promote OSI networking stack
- Model of subject-specific information portals
- Howard provided information and news for crystallographers (with input from Martha Teeter)

1993: gopher – precursor of the Worldwide Web

- Gopher provided “tunnelling” between compatible resource servers
- Operated over OSI (CONCISE) and TCP/IP (WWW) network infrastructures
- Menu-driven
- Provided for different resource types
- Early IUCr experiments at Chester

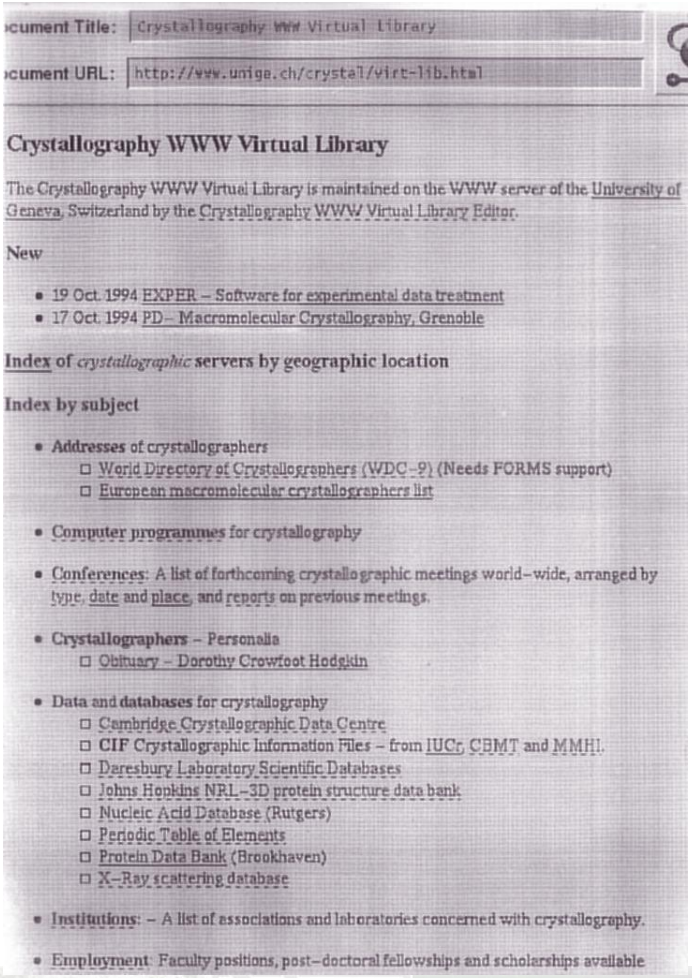
1993: gopher – precursor of the Worldwide Web



1993: mosaic – unleashing the web

- Graphical browser supporting images and text
- 1992: developed by NCSA at U. Illinois Urbana-Champaign
- Released 1993
- Supported http, ftp, nntp, gopher protocols
- Widely credited with popularizing World Wide Web
- 1993/4 Howard moved all crystallography-related content from CONCISE to *Crystallography in Europe* web server at U. Geneva

1993: mosaic – unleashing the web



ocument Title: Crystallography www Virtual Library

ocument URL: http://www.unige.ch/crystal/virt-lib.html

Crystallography WWW Virtual Library

The Crystallography WWW Virtual Library is maintained on the WWW server of the University of Geneva, Switzerland by the Crystallography WWW Virtual Library Editor.

New

- 19 Oct. 1994 EXPER – Software for experimental data treatment
- 17 Oct. 1994 PD– Macromolecular Crystallography, Grenoble

Index of *crystallographic* servers by geographic location

Index by subject

- **Addresses** of crystallographers
  - World Directory of Crystallographers (WDC–9) (Needs FORMS support)
  - European macromolecular crystallographers list
- Computer programmes for crystallography
- Conferences: A list of forthcoming crystallographic meetings world–wide, arranged by type, date and place, and reports on previous meetings.
- **Crystallographers** – Personalia
  - Obituary – Dorothy Crowfoot Hodgkin
- Data and **databases** for crystallography
  - Cambridge Crystallographic Data Centre
  - **CIF** Crystallographic Information Files – from IUCr, CBMT and MMHI.
  - Daresbury Laboratory Scientific Databases
  - Johns Hopkins NRL–3D protein structure data bank
  - Nucleic Acid Database (Rutgers)
  - Periodic Table of Elements
  - Protein Data Bank (Brookhaven)
  - X–Ray scattering database
- Institutions: – A list of associations and laboratories concerned with crystallography.
- Employment: Faculty positions, post–doctoral fellowships and scholarships available

1994: Aperiodic’94 – first scientific conference on the web

https://web.archive.org/web/19970615223724/http://www.unige.ch/crystal/aperiodic/mtg-ch94-index.html

Aperiodic'94

International Conference on Aperiodic Crystals

Les Diablerets, Switzerland 18-22 September 1994

An international cutting-edge conference dealing with recent developments in the study of aperiodic crystals and taking place in the beautiful alpine region of the French-speaking part of Switzerland.

What's New

- Full conference report

Detailed information

- Invited talks arranged by speaker
- Contributions arranged by
  - submission number
  - subject
  - author
  - abstract book
- Conference timetable
- Train timetable
- General
- Conference arrangements
- Submission of scientific contributions
- Registration
- Registration form
- Financial support

Addresses

Before the conference, all correspondence should be addressed to:
Aperiodic'94
University of Lausanne
BSP
CH-1015 Lausanne
Switzerland

Telephone (+41 21) 692 37 71
Telefax (+41 21) 692 36 05
e-mail aperiodic@ic.unil.ch

During the conference mail for participants may be addressed to:
Aperiodic'94
EUROTEL Les Diablerets
CH-1865 Les Diablerets
Switzerland

Gervais Chapuis

1994: W3VL - Crystallography

- World Wide Web Virtual Library arose from an idea of Tim Berners-Lee to create a global, distributed and authoritative resource structuring the information available over the WWW
- Howard removed all remaining content from CONCISE/DISCUS and restructured the Geneva WWW server as the crystallography node of W3VL

1995: ACA Montreal

- Inspired by Aperiodic’94, Yvon LePage used WWW to plan the American Crystallographic Association Annual Meeting
- Collect/disseminate abstracts
- Plan room allocation via online questionnaire

1995: Crystallography World Wide

- A further restructuring to become a community resource
- Job postings, meetings calendar, directories of companies, organizations, facilities, book reviews
- Awareness of other crystallography web servers (SinCris, IUCr) and efforts to minimise overlap

1995: Statistical Descriptors

Acta Cryst. (1989). A**45**, 63–75

Statistical Descriptors in Crystallography

Report of the International Union of Crystallography Subcommittee on Statistical Descriptors*

BY D. SCHWARZENBACH (Chairman), *Institut de Cristallographie, University of Lausanne, BSP Dorigny, CH-1015 Lausanne, Switzerland*, S. C. ABRAHAMS (*ex officio*, IUCr Commission on Crystallographic Nomenclature), *AT&T Bell Laboratories, 600 Mountain Ave, Murray Hill, NJ 07974, USA*, H. D. FLACK, *Laboratoire de Cristallographie aux Rayons X, University of Geneva, 24 Quai Ernest Ansermet, CH-1211 Genève 4, Switzerland*, W. GONSCHOREK, *Institut für Physikalische Chemie der TH Darmstadt, Aussenstelle in KFA/ZFR, Postfach 913, D-5170 Jülich, Federal Republic of Germany*, TH. HAHN (*ex officio*, IUCr Commission on Crystallographic Nomenclature), *Institut für Kristallographie, RWTH, Templergraben 55, D-5100 Aachen, Federal Republic of Germany*, K. HUML (*ex officio*, IUCr Commission on Crystallographic Computing), *Laboratory of X-ray Polymer Structure Analysis, Institute of Macromolecular Chemistry, Czech Academy of Science, 162 06 Praha 6, Czechoslovakia*, R. E. MARSH, *Chemistry Department, California Institute of Technology, Pasadena, CA 91125, USA*, E. PRINCE, *National Bureau of Standards, Reactor Radiation Division, Gaithersburg, MD 20899, USA*, B. E. ROBERTSON, *Department of Physics and Astronomy, University of Regina, Regina, Saskatchewan S4S 0A2, Canada*, J. S. ROLLETT, *Oxford University Computing Laboratory, 8–11 Keble Road, Oxford OX1 3QD, England* AND A. J. C. WILSON (*ex officio*, IUCr Commission on Crystallographic Nomenclature), *University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, England*

(*Received* 28 *March* 1988; *accepted* 2 *September* 1988)

Abstract

The Subcommittee has attempted to elucidate the nature of problems encountered in the definition and use of statistical descriptors as applied to crystallography and to propose procedural improvements. The report contains (*a*) a dictionary of statistical terms established for use by experimentalists; (*b*) a description of the statistical basis for refinement procedures; (*c*) sections dealing with defects in the physical model used for refinement, and with the choice and significance of weighting schemes; and (*d*) recommendations, some of which may be readily implemented, whilst others may require a long-term effort to bring them into general use.

Introduction

A result of several discussions at the XIII International Congress of Crystallography in Hamburg, 1984, particularly those arising at a microsymposium devoted to crystallographic statistics, was a renewed recognition of the wide nonuniformity in use and nomenclature of many statistical methods applied to crystallography. The Commission on Crystallographic Nomenclature addressed this problem soon after the Congress had ended and agreed that an attempt should be made to improve the situation. Accordingly, a Subcommittee on Statistical Descriptors in Crystallography was appointed in early 1985 with its terms of reference 'to examine the validity of current statistical approaches used in estimating the variances in crystallographic quantities and to make recommendations for an improved methodology that rests securely on sound modern statistical theory and that can be widely adopted by the crystallographic community'.

Vigorous correspondence within the Subcommittee resulted in a series of draft reports that gradually evolved toward general consensus. An intermediate report was presented orally at an Open Meeting of the Commission during the XIV International Congress of Crystallography in Perth 1987.

Problems arising from the interface between the mathematical theory of probability and statistics and

* Appointed 27 February 1985 as a Subcommittee of the IUCr Commission on Crystallographic Nomenclature. Following a review by the Chairmen of all relevant IUCr Commissions, the Final Report was accepted on 9 May 1988 by the Commission and on 2 September 1988 by the Executive Committee.

0108-7673/89/010063-13$03.00

Acta Cryst. (1995). A**51**, 565–569

Statistical Descriptors in Crystallography. II.

Report of a Working Group* on Expression of Uncertainty in Measurement

BY D. SCHWARZENBACH (Chairman), *Institut de Cristallographie, University of Lausanne, BSP, CH-1015 Lausanne, Switzerland*, S. C. ABRAHAMS (*ex officio*, IUCr Commission on Crystallographic Nomenclature), *Physics Department, Southern Oregon State College, Ashland, OR 97520, USA*, H. D. FLACK, *Laboratoire de Cristallographie aux Rayons X, University of Geneva, 24 Quai Ernest Ansermet, CH-1211 Genève 4, Switzerland*, E. PRINCE, *National Institute of Standards and Technology, Reactor Radiation Division, Gaithersburg, MD 20899, USA*, AND A. J. C. WILSON (*ex officio*, IUCr Commission on Crystallographic Nomenclature), *St John's College, Cambridge CB2 1TP, England*

(*Received* 18 *August* 1994; *accepted* 15 *December* 1994)

Abstract

The Working Group has examined recent recommendations for evaluating and expressing uncertainty in measurement [*Guide to the Expression of Uncertainty in Measurement*, International Organization for Standardization (ISO, 1993)]. The present publication updates an earlier report of the IUCr Subcommittee on Statistical Descriptors [Schwarzenbach, Abrahams, Flack, Gonschorek, Hahn, Huml, Marsh, Prince, Robertson, Rollett & Wilson (1989). *Acta Cryst.* A**45**, 63–75]. This new report presents the concepts of standard uncertainty, of combined standard uncertainty, and of Type A and Type B evaluations of standard uncertainties. It expands the earlier dictionary of statistical terms, recommends replacement of the term *estimated standard deviation* (e.s.d.) by *standard uncertainty* (s.u.) or by *combined standard uncertainty* (c.s.u.) in statements of the statistical uncertainties of data and results, and requests a complete description of the experimental and computational procedures used to obtain all results submitted to IUCr publications.

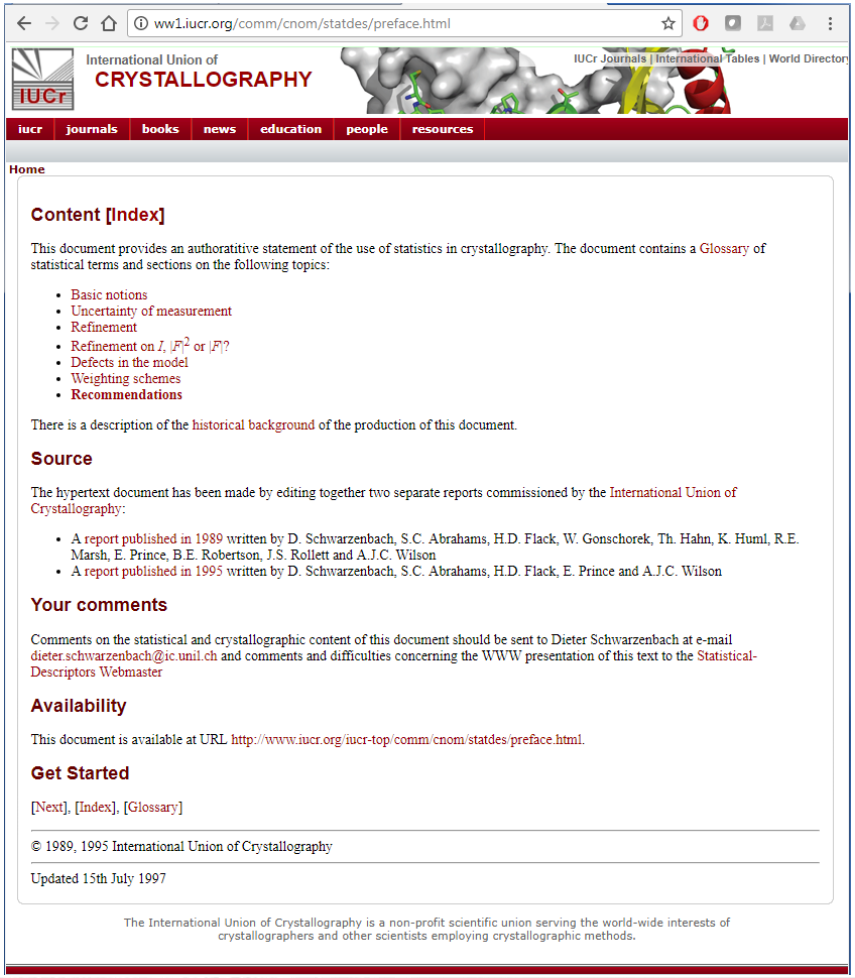
Introduction

The International Organization for Standardization (ISO) has issued a document (ISO, 1993), hereafter referred to as *Guide*, with the purpose of establishing general rules for evaluating and expressing the uncertainty of the result of a measurement. Based on a recommendation of the Comité International des Poids et Mesures, the rules are intended to be applicable to a broad spectrum of measurements. A recent NIST Technical Note (Taylor

* Appointed 4 March 1993 as a Working Group of the International Union of Crystallography Commission on Crystallographic Nomenclature. The final report of the Working Group was accepted on 20 September 1994 by the Commission and 15 December 1994 by the Executive Committee.

Acta Crystallographica Section A
ISSN 0108-7673 © 1995

1995: Statistical Descriptors



ww1.iucr.org/comm/cnom/statdes/preface.html

International Union of CRYSTALLOGRAPHY

IUCr Journals | International Tables | World Directory

iucr | journals | books | news | education | people | resources

Home

Content [Index]

This document provides an authoratitive statement of the use of statistics in crystallography. The document contains a Glossary of statistical terms and sections on the following topics:

- Basic notions
- Uncertainty of measurement
- Refinement
- Refinement on I, $|F|^2$ or $|F|$?
- Defects in the model
- Weighting schemes
- **Recommendations**

There is a description of the historical background of the production of this document.

Source

The hypertext document has been made by editing together two separate reports commissioned by the International Union of Crystallography:

- A report published in 1989 written by D. Schwarzenbach, S.C. Abrahams, H.D. Flack, W. Gonschorek, Th. Hahn, K. Huml, R.E. Marsh, E. Prince, B.E. Robertson, J.S. Rollett and A.J.C. Wilson
- A report published in 1995 written by D. Schwarzenbach, S.C. Abrahams, H.D. Flack, E. Prince and A.J.C. Wilson

Your comments

Comments on the statistical and crystallographic content of this document should be sent to Dieter Schwarzenbach at e-mail dieter.schwarzenbach@ic.unil.ch and comments and difficulties concerning the WWW presentation of this text to the Statistical-Descriptors Webmaster

Availability

This document is available at URL http://www.iucr.org/iucr-top/comm/cnom/statdes/preface.html.

Get Started

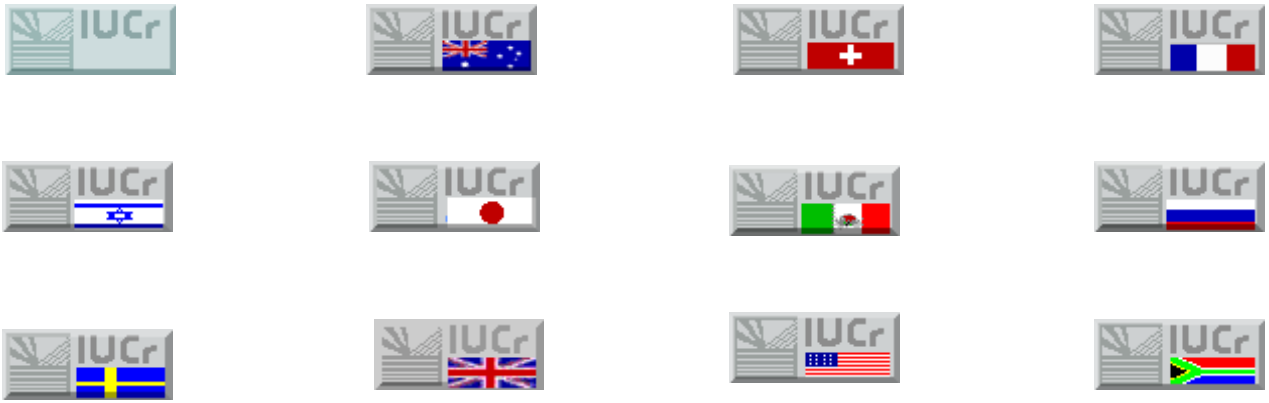
[Next], [Index], [Glossary]

Updated 15th July 1997

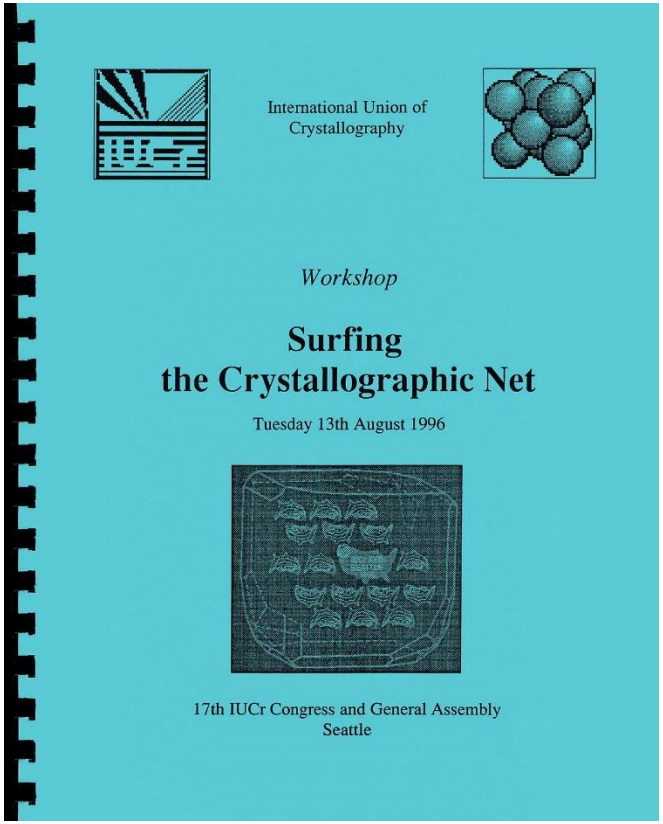
The International Union of Crystallography is a non-profit scientific union serving the world-wide interests of crystallographers and other scientists employing crystallographic methods.

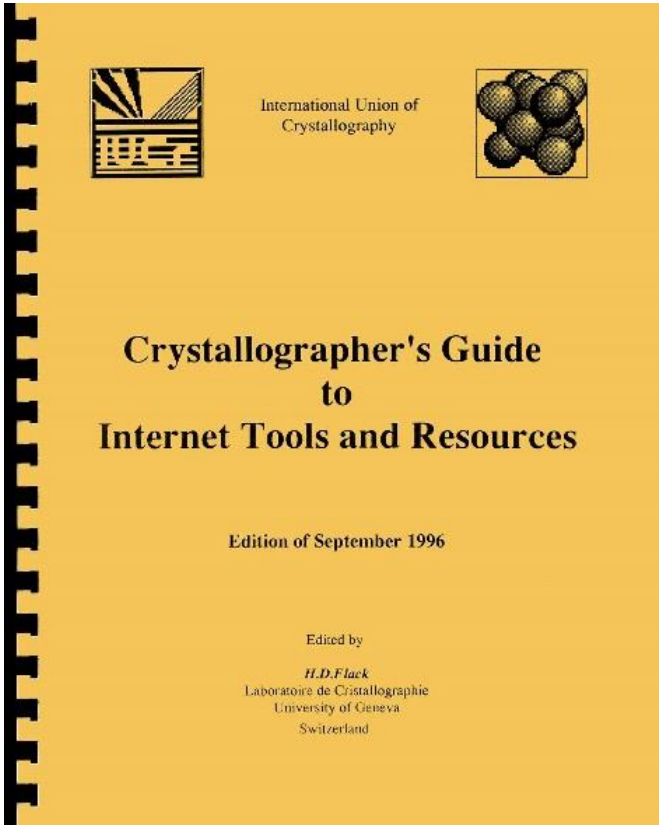
1997: Crystallography truly world wide

- Merger of IUCr content (bm), Crystallography World Wide (Howard Flack) and SinCris (Yves Epelboin)
- Mirroring across the world

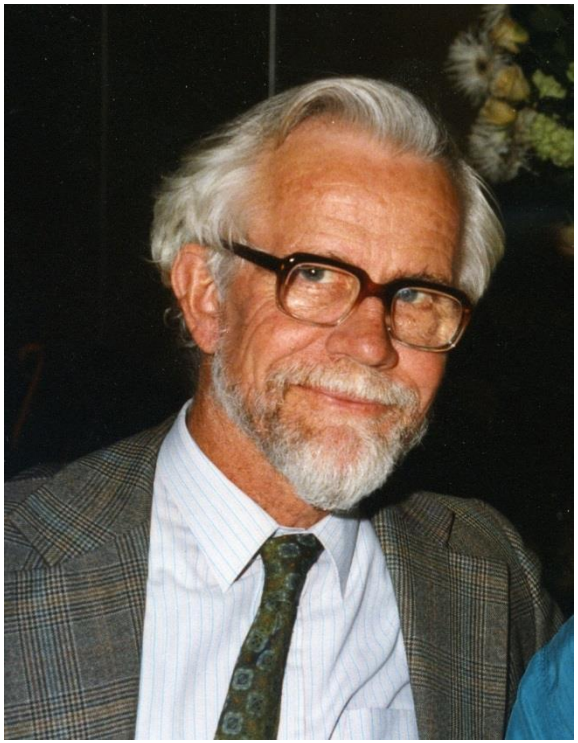


1996: The Crystallographer's Guide



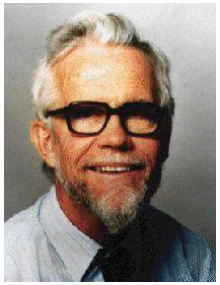


1935-1997: Ted Maslen

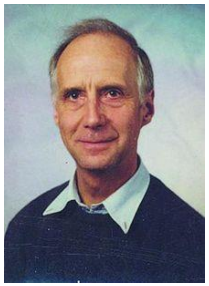


Photographed in 1996, Ted Maslen chaired the IUCr Committee on Electronic Publishing, Dissemination and Storage of Information from 1993 until his early death in 1997, at which point Howard took over until the mid 2000s. The Committee was dissolved in 2009.

Electronic Publishing Committee

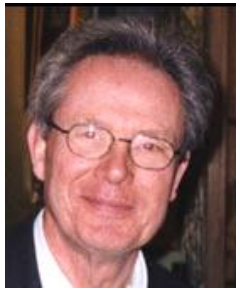


Ted Maslen
STAR/CIF, email, electronic publishing, data checking



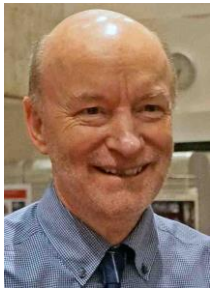
Howard Flack
Distributed information systems, Web, e-mail lists, preprint servers

Lachlan Cranswick
NeXus, mailing lists, web mirrors, Commission websites, newsletters



Yves Epelboin
SinCris, Sofware Database, World Directory of Crystallographers

Simon Parsons
News Online (jobs, meetings, announcements)



Peter Strickland
IUCr Managing Editor

Brian McMahon
IUCr Research and Development Officer

Yves Epelboin, André Authier, Brian McMahon, Howard Flack, Irena Authier at the Authiers' Paris apartment, on the occasion of the Second ICSU–UNESCO International Conference on Electronic Publishing in Science, 19-23 February 1996.

1998: Internet pioneers at the Prague ECM

Howard and CIF

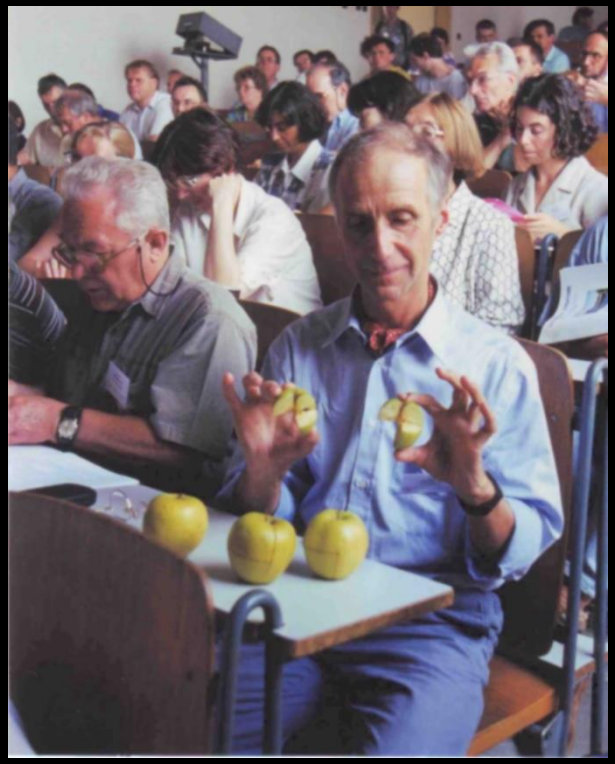
- Impetus for developing a new standard exchange format for crystallography was Howard's challenge to Syd Hall to standardise all diffractometer data
- "Why not SGML?"
- Observer on COMCIFS
- Researches using IUCr CIF archive

Syd Hall
1988 photo coincident with the creation of the Working Party on Crystallographic Information

Other contributions

- 1990-1993 Chair, IUCr Commission on Crystallographic Computing
- 1996-1997 IUCr Representative to CODATA
- 1997-2002 IUCr Representative to ICSTI
- 2001 Input to review process for the Open Archival Information System (OAIS) Reference Model
- 2001 IUCr Journals Archiving Policy

Howard outside the IUCr offices in Chester, 2006. Chester Cathedral in the background.



Howard Flack 1943-2017: a pioneer in electronic publishing

24th Congress and General Assembly
of the International Union of Crystallography
Hyderabad International Convention Centre
21 - 28 August 2017, Hyderabad, India