

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President



Henk Schenk

I cite from a current IUCr press release:

The International Union of Crystallography (IUCr) is excited to announce the availability of 50+ years of groundbreaking crystallographic research on your desktop! The complete text of all IUCr journals back to 1948 is now online. The IUCr is enabling unprecedented access to its complete journal collection. The **Crystallography Journals Online** service (journals.iucr.org) now offers full-text access back to the first issue of all IUCr journals.

More than 50 000 articles have been digitized to create nearly 200 000 PDF pages, all fully searchable on titles and authors. Subscribers holding a current subscription to a particular journal now have online access to all back issues of that journal. Individual articles are also available to nonsubscribers on payment of a fee for each article.

The press release continues with a quotation from Paul Ewald (1888–1985), founding Editor of *Acta Crystallographica*, founding president of the IUCr and pioneer of crystallography: 'Acta is ... a central place for publication and discussion of all research in this vast and ever-expanding field. It borders, naturally, on pure physics, chemistry, biology, mineralogy, technology and also on mathematics.'

So, the back issues of all our journals are online and much earlier than scheduled! The plan was to have the project finished in the spring of 2002, but on 14 November I experimented with the new possibilities of the test version and it was exciting. Now, a month later all is complete and it is a real pleasure to have all articles available at a mouse click. For a lecture, I wanted to go back to the oldest Acta papers on direct methods, and in half an hour I had selected everything I needed and downloaded the original texts to my notebook. So on my way to the AsCA meeting I had my direct methods selection on board — fantastic!

When in Glasgow 1999 Peter Strickland, the Managing Editor of our journals, Brian McMahon, the Research and Development Officer, and John Helliwell, the Editor-in-Chief, proposed the back issue project, the Executive Committee was very positive and gladly allocated the required budget from the Journals Development Fund. At the time it seemed to us a major enterprise that could well take more than the planned two and a half years. But we have a very capable research department at our office in Chester and they designed the whole procedure to be as automatic as possible. So now the IUCr is the only scientific publisher in the world to have all its pages ever printed available online. I'm very proud!

It is mid-December when I'm writing this letter. So this will be my last letter of 2001, a year that finished too quickly. For the IUCr, 2002 will be an important year as we will have our triennial General Assembly and Congress in Geneva. The Congress is the main crystallographic event in three years and will be scientifically of top quality as usual. The General Assembly will discuss the plan for the next triennium, we will decide on the Congress venue for 2008 and many other items will pass the agenda. The Executive Committee will also have intensive discussions with the chairs of the Commissions.

I hope I will meet many of you next August in Geneva. I wish you all the best for 2002, personally and professionally.

Henk Schenk
schenk@science.uva.nl

IUCR ACTIVITIES

COMCIFS reports

COMCIFS is the committee appointed to maintain the Crystallographic Information File (CIF). It includes Subcommittees of the Dictionary Maintenance Groups, the Dictionary Review Committee, the Publicity Committee, the Software Development Committee and the dictionary Definition Language Committee. Currently under final review are the modulated structure dictionary (msCIF) and a dictionary containing basic symmetry concepts used in crystallography (symCIF). Draft dictionaries for electron density (rhoCIF), magnetic structures (magCIF) and small angle scattering (sasCIF) were submitted to the Dictionary Review Committee and are currently undergoing revision to bring them into conformity with CIF standards. Protocols for merging two or more dictionaries into a larger virtual dictionary and developing the necessary software for manipulating CIFs are currently major concerns.

Most of the software currently available for CIF is in the form of toolboxes to help others write CIF applications. The program enCIFer, to be released by the Cambridge Crystallographic Data Centre in late 2001, has many features that crystallographers will find useful. These include a browser that provides clear error markup, an alphabetic view of data names, data entry panes containing the dictionary definitions, buttons for the special character sequences frequently used in CIF text, spreadsheet loop displays, text searching, a text editing window, user templates and a crystal structure visualizer. Several members of COMCIFS are working on the text for Volume G of *International Tables for Crystallography*, the volume that describes the CIF standards. As a result of the efforts of J. Westbrook, D. Greer and others, mmCIF has been recognized by the Object Management Group as providing the Common Object Request Broker Architecture standard (CORBA) for the exchange of macromolecular information between databases.

An exciting proposed extension for CIF is a dictionary of Relational Expression Language (dRel) which will provide algorithmic expressions that allow values for each item in the dictionary to be derived from other items, e.g., the calculation of the density from the cell mass and cell volume. A preliminary account of dRel has been given by Spadaccini, Hall and Castledean (2000) *J. Chem. Inf. Comput. Sci.* **40**, 1289-1301.

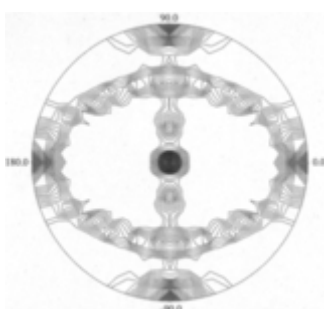
I.D. Brown, Chair

IUCR JOURNALS NEWS

Molecular replacement: finding the right search model

Acta Cryst. (2001). D57

The October 2001 issue of *Acta Cryst.* Section D (volume D57, part 10) is the collected proceedings of the annual CCP4 Study Weekend held this January at the U. of York, UK, and entitled 'Molecular replacement and its relatives'. The most frequent stumbling block to successful *ab initio* solution of a macromolecular crystal structure by molecular replacement is low structural similarity between the search model and the target structure, and many of the articles addressed this important problem of finding the optimal search model. Owing to space constraints, this is a personal selection of articles that highlight this theme.



It is helpful to inspect visually the internal symmetry of the molecule in the crystal for comparison with the EM image. The figure shows the self-rotation function for the X-ray image of the bacteriophage SPP1 portal protein showing that the peaks are consistent with expected 13-fold rotational symmetry of the EM image.

Any improvement in the success rate of molecular replacement methods will clearly have an impact on the outcome of the structural genomics projects now underway or planned, given that a significant proportion of the proteins coded by a genome are likely to contain previously unknown folds, or folds having very low structural similarity with known structures.

In 'Pushing the boundaries of molecular replacement with maximum likelihood' Randy Read demonstrates how his new 'BEAST' program utilizes a likelihood-based scoring function that can compensate for a poor model. Likelihood-based scoring functions, which measure the probability that the values of the experimental observations (in this case the X-ray diffraction intensities) would have been obtained if the current model were correct, are now used routinely in model refinement, and their use in molecular replacement is a logical extension of this. The author shows that combining multiple models, weighing them according to their likelihood of similarity with the target structure provides improved results.

On the subject of model quality, in 'Molecular replacement by evolutionary search' Charles Kissinger reports that polyalanine models are frequently better as search models for protein structures than ones that include side-chain atoms, even when the co-ordinates of those atoms are known quite accurately (though normally less accurately than those of the main-chain atoms). This may seem somewhat counter-intuitive, but is in accord with a common observation that less complete but more accurate models are often better than more complete but less accurate ones.

Other articles focus on less traditional types of molecular replacement model, both structural and non-structural (such as an electron density map or a molecular envelope), including models obtained by NMR, EM or solution scattering techniques.

In 'Molecular placement of experimental electron density: a case study on UDP-galactopyranose mutase' Jim Naismith describes use of the subunit-averaged electron density from a $P2_1$ crystal form of the enzyme as a molecular replacement model for a $P2_12_12_1$ crystal form. The relationship between the crystal forms so obtained allowed use of multiple crystal averaging to solve the structure.

In 'Phasing from an envelope' Quan Hao describes the use of molecular envelopes determined from low-resolution X-ray scattering data from a protein in solution to orient and position the molecule in the crystal by a real-space search technique.

In 'Using electron-microscopy images as a model for molecular replacement' Eleanor Dodson reviews the technical problems associated with using EM models for *ab initio* solution of crystal structures by molecular replacement. Not the least of these problems are the widely varying conventions for describing data structures (in particular those for electron density maps) used by electron microscopists and X-ray crystallographers!

In 'NMR trial models: experiences with the colicin immunity protein Im7 and the p85 α C-terminal SH2-peptide complex' Richard Pauptit describes the non-trivial solutions of two protein structures using ensemble NMR models from which the more flexible portions have been excised. In a similar vein, in 'Solution solution: using NMR models for molecular replacement' Yu Wai Chen describes a protocol for preparation and use of NMR-derived models and results of its application.

Finally, two articles assess the potential of using all available deposited structural information, directly or indirectly to develop better search models. In 'Creating structure features by data mining the PDB to use as molecular-replacement models' Tom Oldfield concludes that more advanced molecular replacement techniques than those currently available will be required to allow use of protein fragments derived by data-mining techniques as search models.

In 'Evaluating the potential of using fold-recognition models for molecular replacement' David Jones analyses all the structures in the PDB solved by molecular replacement in order to assess the minimal degree of structural similarity required for successful solution, and then goes on to use this as a yardstick to judge the current potential of tertiary structure prediction and threading methods to generate useful molecular replacement models. He attempts to estimate the potential impact of these methods on the success rate of a typical structural genomics project, arriving at an estimate that about 50% of the protein structures from a 'typical' genome will be soluble by a combination of structure prediction, modelling and molecular replacement.

This issue of *Acta Cryst. D* provides a comprehensive update of current work in this field, whose overall strategic value will be immense when the goal of 'complete coverage of all the protein folds' is realised. This goal is a major funded objective of the NIH structural genomics initiatives in the USA.

Ian Tickle, Astex Technology Ltd, Cambridge, UK

AWARDS AND PRIZES

News from ICDD

Goehner and Michael Receive Hanawalt Award



The Int'l Centre for Diffraction Data (ICDD) takes pleasure in announcing that Raymond P. Goehner, and Joseph R. Michael, both of Sandia National Laboratories, Albuquerque, New Mexico, USA received the 2001 J.D. Hanawalt Award for excellence in the field of X-ray powder diffraction at the 50th Annual Denver X-ray Conf. in Steamboat Springs, Colorado, USA, August 1, 2001. Goehner and Michael presented the Hanawalt Award Lecture entitled, 'Phase Identification Using Electron Backscatter Diffraction in the SEM: A Powerful Tool for Materials Science'.

The J.D. Hanawalt Award is presented every three years for important contributions to the field of X-ray powder diffraction and phase identification published within the last five years. The award consists of a plaque, an honorarium, and travel funds to attend the meeting at which the award and lecture will be presented.

Previous recipients include: Herbert Göbel, 1998; Daniel Louër, 1992; William Parrish, 1986; and Ludo K. Frevel, 1983.

Appointment of new executive director

The ICDD is pleased to announce that Tim Fawcett is the new Executive Director of the ICDD. Tim has been a long time ICDD member, ICDD Fellow, and member of the Board of Directors (1986-1988).

Tim received his BS degree with honors from the U. of Massachusetts, and his Ph.D. in Inorganic Chemistry from Rutgers U. in 1979. He joined Dow Chemical Co., worked in the X-ray diffraction facility, managed the inorganic analysis laboratories and from 1989 to 1994, he was a manager in Dow's Ceramics and Advanced Materials Laboratories. Since 1994 he has managed Dow's Advanced Technologies and Inorganic Coating Group, the Interfacial Sciences Discipline, and most recently, two of Dow's new product development areas which involved a portfolio of projects leading to advanced materials products.

AWARDS AND PRIZES**BCA prize**

The British Crystallographic Assn Council has approved a 'BCA Prize Lecture' named in honour of a prominent British crystallographer (the name would change with each award) and awarded to any crystallographer in the world. There should be a link between the work of the two people involved.

The crystallographer in whose honour it is given would attend the BCA Meeting and present the prize, with expenses paid for by the BCA. The recipient would give a lecture at the BCA Meeting and receive a trophy and full travel costs.

Chris Gilmore, BCA Crystallography News, June 2001

AWARDS AND PRIZES

ACA Trueblood award

A decision was taken at the April ACA Council Meeting to establish a new ACA award in honor of Ken Trueblood. The Council considered ideas and solicited input from a number of people with connections to Ken. The establishment of the Trueblood Award in Chemical or Computational Crystallography was announced at the Los Angeles meeting.

NOTICE

Honors

- **Kenneth N. Raymond** (U. of California, Berkeley) is among the new members of the American Academy of Arts & Science for 2001
- **Julia Goodfellow**, currently head of crystallography at Birkbeck College, London, will become the first woman to lead the Biotechnology and Biological Sciences Research Council.
- *Fellows of the Royal Society* Congratulations to **Andrew Leslie** and **George Sheldrick** who have been appointed Fellows of the Royal Society.
- **Ada E. Yonath**, Martin S. Kimmel Professorial Chair, Weizman Inst. of Science, Rehovot, Israel, will receive the *2002 F.A. Cotton Medal* sponsored by the ACS Texas A&M Section and the Texas A&M U. chemistry dept. Yonath was chosen for her pathbreaking research elucidating the structure and function of ribosomes.
- The recipient of the *2001 ENSA/Hälg Prize* is **Jane Brown**, Inst. Laue Langevin, Grenoble, in recognition of her outstanding contributions to the science of neutron scattering over the last four decades. The prize was presented at a special session of the Int'l Conference on Neutron Scattering in Munich in September.
- Massachusetts Inst. of Technology biophysicist **Alexander Rich** has been selected to receive Sigma Xi's *2001 William Procter Prize for Scientific Achievement*. Sigma Xi's highest honor, the annual Procter Prize, recognizes scientific achievement and an ability to communicate the importance of that research to others. Rich has long been recognized as a preeminent researcher in structural molecular biology. In 1979 he led a team of researchers at MIT that startled the world of structural biology with the announcement that they had found a 'left-handed' form of DNA. Rich described in *Science* (June 11, 1999) how the three-dimensional structure of ZDNA binds to proteins involved in editing genetic messages important in a number of brain receptors. Rich received the US Medal of Science in 1995.

NOTICE

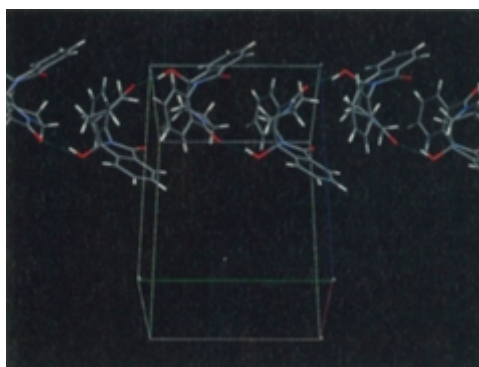
Hodgkin laboratory - a landmark

The former laboratory of Nobel Laureate Dorothy Crowfoot Hodgkin has been designated as a Chemistry landmark at a UK Royal Society celebration chaired by Graham Richards, the Chairman of the Dept of Chemistry in Oxford. T. Ledwith of the Royal Society of Chemistry presented a memorial plaque that now hangs on the archway of the main entrance to the Inorganic Chemistry Laboratory in South Parks Road. The inscription reads:

'In this building from 1956-1994 and at other times in the Oxford Science Area, professor Dorothy Crowfoot Hodgkin (1910-1994) OM, FRS, Nobel Laureate, led pioneering work on the structures of antibiotics, vitamins and proteins, including penicillin, Vitamin B12 and insulin using X-ray diffraction techniques. Many methods for solving crystal structures were developed taking advantage of digital computers from the very earliest days. The work provided a basis for much of present day molecular structure driven molecular biology and medicinal chemistry'.

NOTICE

The Cambridge Structural Database: a quarter of a million crystal structures



On October 5 2001, the 250,000 crystal structure was archived to the Cambridge Structural Database (CSD), marking another milestone in the ever-accelerating growth of the world's repository of organic and metal-organic crystal structures.

The 250,000th structure is an organic compound, the product of a photocyclization reaction. It has been assigned the CSD reference code IBEZAQ and was one of two structures published in *Angewandte Chemie* (Int'l Edition), 2001, **40**, 577-579. The paper's authors are A. G. Griesbeck, W. Kramer, and J. Lex, of the U. of Köln, Germany. 'This is a landmark achievement, not only for the CSD, but also for small-molecule crystallography worldwide,' said F. Allen, Scientific Director of the Cambridge Crystallographic Data Center (CCDC). The CSD began in 1965 with just a few hundred structures. We expect to reach half a million structures by 2010.



CSD staff Steve Maginn, David Bardwell, and Ian Bruno at the ACA Annual Meeting in Los Angeles, July 2001.

The CSD has subscribers at almost 120 industrial sites and nearly 1000 academic institutions, covering 56 countries worldwide. 'Expansion, maintenance, development, and distribution of the CSD and its associated software continue to be the cornerstones of the CCDC's activities,' said D. Hartley, CCDC's Executive Director. 'We are not only determined to maintain the currency of the CSD itself, but also to enhance its permanent value through the development of new scientific applications and software products.' The CCDC and its collaborators also develop CSD-related application programs such as SuperStar and GOLD, for investigating protein-ligand interactions, for protein-ligand docking, and for DASH, a program for Structure solution from powder diffraction data. A parallel database system; Relibase+, is also available for the Analysis of Protein-ligand structures in the Protein Data Bank. For further information, contact: S.J. Maginn, Support and Marketing Manager, CCDC, FAX: 44 1223 336066; maginn@ccdc.cam.ac.uk, www.ccdc.cam.ac.uk/.

MISCELLANY

Crystallography and antiquities

Diffraction can be employed to investigate the pigments used to decorate ancient Egyptian coffins and other artifacts and to determine how the artist's palette varied in different parts of Egypt and the ways in which it changed over time. X-ray powder photography was used more than sixty years ago, by Joep and Huse (1940), to characterize a series of samples of Egyptian Blue, used on many ancient artifacts. Egyptian Blue, a copper calcium silicate, which is identical to the mineral, cuprorivaite; it was used widely across the ancient world from 3100 BC up until the 9th century AD.

Andrew Middleton, The British Museum , BCA Crystallography News, No. 78

AWARDS AND PRIZES

Sidhu award

The Sidhu award for 2001 was presented to Laurence Sheppard of the Dept of Psychology and Biophysics at Mount Sinai School of Medicine of New York U. at the 59th Pittsburgh Diffraction Conference, which was held in Cincinnati, Ohio in October, 2001. Sheppard is engaged in a number of studies of structural biology including the structure of Tubby, a mouse protein implicated in obesity.

The award is made in memory of Dr. Surhain Sidhu, Prof. of Physics and Director of the X-Ray Lab at the U. of Pittsburgh, and a founder of the Pittsburgh Diffraction Conference in 1942. At Argonne National Lab, Prof. Sidhu pioneered the use of the null matrix technique in neutron diffraction. This technique involves choosing isotopes in the proportion that gives a zero net coherent scattering factor, and it has been widely used for studying biological materials in which the H:D isotopic ratio is appropriately adjusted. The award recognizes an outstanding contribution to crystallography or diffraction research by an investigator whose doctoral degree was conferred within five years before the award date.

Previous Sidhu Award winners

1999 Changill Ban & M.C. Wahl
 1996 M. J. Regan
 1995 M. Georgiadis
 1994 A. Vrielink & J. Wang
 1993 M. Pressprich & T. Yeates
 1992 R. C. Stevens
 1990 L. Brammer
 1989 M. Luo
 1988 Q. Shen
 1986 D. Agard & J.M. Newsman
 1985 D.C. Rees
 1980 G. Petsko
 1978 K. Hodgson & G. DeTitta
 1975 P. Argos
 1974 B.C.Larson & N.C. Seeman
 1972 D.E. Sayers
 1971 L.K. Walford
 1970 S.H. Kim
 1969 T.O Baldwin
 1968 R.M. Nicklow
 1967 A.I. Bienenstock

REGIONAL NEWS

At Daresbury SRS

Recent results from beamline 2.1 at the Daresbury SRS suggest the X-ray fiber diffraction can be used as a diagnostic method for the investigation of cancer tumors in breast tissue. The study, which was published by Lewis, *et al.* (*J. Synch. Rad.* 7, 348), shows clear differences between fiber diffraction patterns recorded from healthy and diseased breast tissue. These differences are believed to occur as a result of changes in the structural ordering of the collagen within breast carcinogens. Collagen is a major component of the intracellular matrix (ECM) in breast tissue; its degradation is known to be of major importance in the morbidity and mortality of cancer.

Also at Daresbury, Langan, Nishiyama, and Chanzy (*J. Am. Chem. Soc.* **121** (43), 9940) are using neutron fiber diffraction to study hydrogen bonding in cellulose, one of the most abundant polymers on Earth. The maps clearly show the liable hydrogen atoms involved in the hydrogen bonding and allowed the authors to distinguish between two competing models for cellulose II.

BCA Crystallography News, No. 78

REGIONAL NEWS

MSA goes international

Past and future developments



Of the 2100 individual members in the MSA, 41% are non-US residents. The MSA has expanded representation on its committees to include many members from abroad. Ian Parsons, of the Dept of Geology and Geophysics, U. of Edinburgh, was the first Mineralogical Society of America's (MSA) Distinguished Lecturer who did not reside in North America. The first short course organized by the MSA in a country outside North America, was held in Cambridge, England in 2001. The MSA will co-sponsor the 18th General Meeting Int'l Mineralogical Assn (IMA), in Edinburgh, UK in September, 2002. For the year 2001 Endowment Fund of MSA's total contributions now stands at \$19,663.00 which is an increase of \$6,742.00 (52%) over last year, 23% of which was from abroad. At the Annual Meeting of the Geological Society of America in early November, 2001, the Awards Luncheon, the Roebling Medal will be awarded to Peter J. Wyllie, the MSA Award will be given to Peter C. Burns, and the Distinguished Public Service Medal will be presented to Jeffrey E. Post. The Spring MSA-Sponsored meeting will be in conjunction with the American Geophysical Union meetings in Washington where the second Dana Medal will be awarded to Michael F. Hochella, Jr.

Cornelis ('Kase') Klein, MSA President

NOTICE

FreeWare



Lachlan Cranswick, curator of a collection of freely available crystallographic software was among the speakers in a symposium on Diffraction Methods in Undergraduate Studies at the 2001 ACA meeting in Los Angeles. (left to right) V. Young, W. Clegg, T. Proffen, L. Cranswick, A. Hunter, K. Kantardjieff, W. Cordes, J. Glusker, and R. Sparks.

In the Computer Corner of the December 2000 issue of the *Newsletter of the IUCr Commission on Powder Diffraction*, L. Cranswick presents a list of freely available crystallographic and powder diffraction software, including CRYSFIRE for DOS/Windows Powder Indexing Suite by R. Shirley, CHEKCELL for Windows powder indexing helper tool by J. Laugier and B. Bochu, EXPGUI for Windows and Linux Graphical User Interface to GSAS by B. Toby, New DBWSTOOL – Graphical User Interface for Windows Over DBWs by Bleicher, Sasaki, and Santos, GUF1 for DOS Shareware for Powder Diffraction Measurements and Evaluation by R. Dinnebier, New RIETAN2000 Rietveld Refinement Program by F. Izumi, New GRETEP (Grenoble Thermal Ellipsoids Plot Program) for Windows by J. Laugier and B. Bochu, Planton and Addsym: Published Example of Finding Missing Symmetry Using the Addsym Function Within, by T. Speks, Platon, Crystals for Windows Single Crystal Suite for Structure Refinement and User Friendly DLS (Distance Least Squares) by D. Watkins, R. Cooper and co workers, New GPL'd ESPOIR 3.5 for Windows by A. Le Bail with Tutorial on Setting up Within 10 Minutes to Solve an Organic Structure from Powder Diffraction Data. Further information and how to access and download these programs can be found at www.iucr.org or <http://bragg.ing.unitn.it/cpd/Newsletters/index.html>. If you wish to be added to the CPD Newsletter mailing list or have changed address, contact the Chairman or send an e-mail to CPD@ing.unitn.it.

CPD News, No. 24, Dec. 2000

NOTICE

PDB at a glance



Since the beginning of the year 2001, 1123 structures have been deposited to the Protein Data Bank – 80% were determined by X-ray crystallography. 89% are proteins, 4% are protein-nucleic acid complexes, and 7% are nucleic acids. (Figures updated on 5/17/01).

New features have been added to the reporting features available at the PDB. The MICE collaborative molecular viewer permits remote users to share a VRML-based view of a molecule via the Internet.

Further details can be obtained by visiting the MICE web site at <http://mice.sdsc.edu/> or by clicking on the help link accessible from the View Structure page.

Additionally, a new feature has been added to the beta site that allows PDB users to create their own customized tabular reports. By selecting 'Create A Tabular Report' from the option scroll bar at the top of the Query Result Browser page, users can choose from a variety of parameters that will be used to generate a report from a result list.

Christine Zardecki, PDB Rutgers

NOTICE

Web courses

Two distant learning courses are provided from CNRS laboratories at the U. du Maine (France). The QTA Internet Course (Quantitative Texture Analysis) coaches the students from diffraction to quantitative texture-microstructure analysis to properties (<http://lpec.univ-lemans.fr/qta>). The SDPD Internet Course (Structure Determination by Powder Diffractometry) teaches how to obtain a crystal structure in absence of a suitable single crystal (<http://sdpd.univ-lemans.fr/course>). Both courses are asynchronous. Registration is open at any time.