

COMMISSION ON POWDER DIFFRACTION

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

NEWSLETTER No. 12, APRIL 1994

Is Anybody Out There? : World Wide Crystallographic Netnews/Usenet Newsgroup on the Internet - "sci. techniques. xtallography".

Electronic networks are becoming increasingly important to science in overcoming the large distances and time differences between researchers. The most important network for scientific communication is the Internet (International Academic and Research Network) which is so large, its size cannot be accurately determined. Most scientific users of this network would know of it for providing services such as E-mail, Telnet and FTP. However, there are other "free" services created to benefit scientists. A newly created service directly relevant to crystallographers is the crystallography newsgroup (sci.techniques.xtallography).

The "Usenet" is a giant electronic bulletin board system (BBS) provided on the Internet that allows discussion on over 2,500 topics (or newsgroups). Its speed and availability make it a potentially powerful scientific resource. "Posting" a message on a newsgroup (which is similar to e-mail) only takes hours to travel world wide to all other computers linked to the internet. These "articles" can then be read or "followed up" by posting a reply that can be read by any interested people. This procedure is, for most people, done by public domain "news-reading" software available on most computers connected to the Internet.

In October of last year, a crystallography newsgroup (sci.techniques.xtallography), was created after a successful Usenet vote. This newsgroup allows crystallographers an easy way of discussing crystallographic topics and queries in near real time. Articles on the newsgroups only last 2 to 14 days on most computer systems but an archive of articles in an ascii "e-mail" format is available via anonymous ftp (sol.dmp.csiro.au:/pub/xtallography).

Although this newsgroup was only formed in October 1993, it is already popular as a discussion forum for problems and ideas. Conversations may be carried on

about theoretical or practical topics. The important feature is that the response that is the most helpful may come from someone that you would not have considered asking. The potential is limitless. With normal e-mail, your message must be directed at a specific recipient; but when using the newsgroup, you have the opportunity to query everyone in the group.

Some of the topics which were considered when the newsgroup was formed include:

- Powder diffraction (X-ray and neutron)
- Electron diffraction
- Single crystal diffraction
- Rietveld refinement
- Software
- Databases
- Data formats
- Hardware/equipment
 - Alignment and calibration
 - Trade or sale of old apparatus
 - Source of specialized equipment
- Phase identification and quantification
- Sample preparation techniques
- Sources of materials and compounds
- Announcements
- Pre-review of articles
- Accuracy and validity of results
- Positions wanted or available

Obviously, the list is endless. There are some things for which a newsgroup is not an appropriate forum. It is not an alternative to publication of structures or articles to bypass the peer review procedures. Nor should it be a forum to expound on philosophy rather than science.

To find out how to participate in this newsgroup, contact your librarian or systems manager. Alternatively, more information

can be obtained by contacting Lachlan Cranswick of the CSIRO Division of Mineral Products in Melbourne, Australia (E-mail : lachlan@dmp.csiro.au or Fax : +61-3-646-3223. This newsgroup is "unmoderated" meaning no-one actually runs or administers it, and is open to anyone who wishes to apply it to their research or general crystallographic interests. Everyone is thus welcome and invited to make use of this facility. Given the announcements of new "information highways" in Europe, USA and Japan, electronic communications of this type will have a much higher profile in the future.

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- 4) Borman, S. (1993) Chemical and Engineering News, Oct 11, pp 26-27.
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NEWS FROM THE CPD CHAIRMAN

The next three years should see the CPD continue its tradition of being one of the more active "working" Commissions in the IUCr. We have a very healthy, if not exhausting portfolio of ongoing and new projects that are a reflection of the very diverse range of activities underway in the broad community of powder diffractionists. These projects are listed below. The CPD welcomes the participation of readers in all of these projects.

In addition, the CPD is involved in the organisation and/or support of a number of conferences and workshops between now and the next IUCr Congress in Seattle in 1996. We welcome any suggestions that you might have for additional meetings but, in view of the number of proposals already on the drawing board, any new proposals would be best scheduled for the post Congress period. Our early warning of these proposals will enable us to coordinate these activities with other groups who might be making

similar plans.

Ongoing projects of the CPD from the 1990-93 triennium include the following:

Biannual issues of the CPD Newsletter, with rotating Editorship by members of the CPD.

Phase II of the Powder Diffraction Program Information Exchange Bank (PIXB), co-produced by CPD member Prof. Deane Smith of the Pennsylvania State University and Dr. Syb Gorter of the University of Leiden, The Netherlands.

Phase II of the Rietveld Refinement Round Robin, convened by CPD Chairman Dr. Rod Hill; the results have been accepted for publication in the Journal of Applied Crystallography.

International Conference on "Powder Diffraction and Crystal Chemistry", St. Petersburg, Russia in July, 1994, organised under the auspices of the Russian State Committee on Higher Education, the Ministry of Science, Higher School and Technical Policy, the Russian Academy of Sciences and the Academy of Natural Sciences of Russia (PDR-94). CPD member Dr. Jaroslav Fiala is the Chairman of the Scientific Program Committee.

An International Workshop on "Advanced Powder Diffraction Techniques in Mineral and Materials Processing", Pretoria, South Africa, October 1994, organised by the South African Crystallography Society and the Mineralogical Association of South Africa (PDSA-94). CPD member Dr. Lynne McCusker is the Chairman of the Scientific Program Committee.

Support for the Workshop on "Ab-initio Determination of Crystal Structure from Powder Diffraction Data", Oxford in July, 1995, organised by Dr. Bill David of the Rutherford Appleton Laboratory, UK

A survey on the determination of crystallite size and microstrain from powder diffraction data, co-organised with the ICDD, and run in conjunction with the "International Conference on Powder Diffraction", Liptovsky Mikulas, Slovakia, August 1995 (PMCS-95). CPD member Dr. Jaroslav Fiala is the Chairman of the Scientific Program Committee. This project may

be developed into a Round Robin.

New projects identified for attention during the 1993-96 triennium include:

A Round Robin on Quantitative Phase Analysis from powder diffraction data, convened by Prof. Deane Smith of the Pennsylvania State University and Dr. Rod Hill of the CSIRO Port Melbourne, Australia.

A Microsymposium on Powder Diffraction at the 1996 IUCr Congress and General Assembly in Seattle (MSPD-96).

A Satellite Meeting on Powder Diffraction associated with the 1996 IUCr Congress, possibly to be held in Denver and jointly organised by the CPD and the Denver X-ray Conference Office (SMPD-96).

General News:

I am pleased to announce that the IUCr Executive Committee has approved the recommendation of the CPD that Dr. Daniel Louër be appointed as Secretary for the 1993-96 triennium. We also welcome the news that the EC has approved the appointment of Prof Ray Young and Dr. J. Ian Langford as Consultants to the CPD for the same period.

Before closing this short update on current CPD activities, I must take this opportunity to express the gratitude and admiration of the CPD members to Ray Young for his superb Chairmanship of the CPD during the first two triennia of the CPD's existence, from 1987-1993. The past six years have been extremely active for the CPD, and this effort has been due in no small measure to Ray's outstanding leadership and enthusiasm. His perseverance and high-level of organisational skills has been central to the success of all of the projects that have been executed by the CPD during the past six years, and his legacy of on-going projects will ensure that his influence will continue to be felt for some time to come. In this regard, we all very much welcome his continued activity and influence as a CPD Consultant for the next three years.

R.J. Hill
CPD Chairman

PROPOSED ROUND ROBIN PROJECT ON QUANTITATIVE PHASE ANALYSIS

Along with the continued advancements in the determination and refinement of crystal structures using powder diffraction data, there are also extensive developments in quantitative phase analysis using powder diffraction data. There are many phase analysis situations where diffraction methods offer the only practical solution to the problem, thus there is renewed interest in the application of modern analysis techniques to an age old question.

The difficulties of quantification by diffraction methods in the past have been the limited accuracy available when using individual peaks or peak clusters in the analysis. Consequently, many potential users have avoided the technique and tried alternative approaches. In the last ten years, whole pattern methods have been developed to eliminate the difficulties of decomposing the peak overlaps to acquire the necessary intensity information when using a limited number of peaks. Whole-pattern fitting, Rietveld analysis and combinations of these methods have shown considerable promise toward improvement of accuracy. With the increased application of these new approaches, it is now time to test the new procedures to determine the limiting factors which affect the accuracy under a variety of conditions concerning the nature of the samples and the instrumentation.

During this next triennium, the CPD will be organizing and initiating a round-robin project on phase quantification by diffraction methods. The project will be designed to test the preparation of samples, the collection of the data, and the analysis of the data by the variety of programs that are available. This announcement is meant to initiate input from interested individuals concerning design of the project. We would appreciate suggestions as to the types of tests that should be performed and the types of samples that should be included. We would also like to hear from potential participants who would be interested in performing the necessary tests.

Input may be directed to Deane Smith, Department of Geosciences, The Pennsylvania State University, University Park, PA 16802, USA. FAX: +1-814-863-7845; E-mail SMITH@VAX1.MRL.PSU.EDU.

The Spring-8 Project: a new facility for synchrotron radiation in Japan

Spring-8 (Super Photon Ring with a 8 GeV storage ring) is the name of a new facility for synchrotron radiation, which is now under construction in Nishi-Harima (west of Osaka), Japan. The first photons will appear in 1998, and then it may be put on-line for outside users. The Japanese government (Science and Technology Agency) has initial plans to construct ten public beam-lines by the year 1998; and the project team, consisting of the people in The Institute of Physical and Chemical Research (RIKEN) and Japan Atomic Energy Research Institute (JAERI), is working toward this goal. Then, a third party (JASRI) will take over the project, and an additional 20 public beam-lines will be constructed hopefully within a few years after 1998. The final facility, as proposed today, will have (possibly) 61 beam-lines (38 insertion devices and 23 bending magnets).

The facility is being constructed in a new town on the mountain side of Nishi-Harima. The storage ring with a circumference of 1436 m surrounds the top

of a mountain. About 10% of the building construction for the ring is completed at present, and another 36% is under construction. An aerial view shows one third of the building with shining silver roof. The construction of the remaining part of the building will be started in the 1994 fiscal year.

In May 1993, the Users' Association was established, and it now has about 800 members. At present, thirty three subgroups have introduced their names as candidates for the user groups of individual beam-lines. The author of this news is in charge of the construction of a beam-line called "High-Resolution Powder and Thin-Film Diffraction". As you can see from the name of beam-line, one future experimental station will be used for high-resolution diffraction studies for powder and thin-film structure analyses. Presently, individual subgroups are competing with each other for using the first ten public beam-lines. More concrete news will be delivered after one or two years.

Hideo Toraya
Ceramic Research Laboratory
Nagoya Institute of Technology



• EPDIC-3

The Third European Powder Diffraction Conference, Vienna, Austria, 23-27 September 1993.

More than 300 participants from 25 different countries took part in the Third European Conference on Powder Diffraction, which was organized by Prof. A. Priesinger at the Technical University of Vienna. The conference was sponsored by The Austrian Committee of Crystallography and Österreichische Mineralogische Gesellschaft.

The meeting started with a Workshop on the Powder Diffraction File (JCPDS/ICDD) and was followed by three intense days of main lectures, oral presentations and poster sessions. The first EPDIC award was handed over to Dr. Maurizio Bellotto from CSIE Technologie Innovative, Milan, Italy, who gave an award lecture on "High temperature phase transitions in kaolinite: the influence of disorder and of kinetics on the reaction path".

The main lectures covered a wide range of useful applications of the powder diffraction technique from "Angle dispersive powder diffraction at high pressure" by Dr. Malcolm McMahon, University of Edinburgh, UK to "Neutron powder diffraction and magnetic structures" by Dr. Francoise Bouree, Laboratoire Leon Brillouin, Saclay, France. Another highly appreciated lecture was given by Prof. Pekka Sourtii from Helsinki University, Finland, at present responsible for the design of the powder instruments at the European Synchrotron Radiation Facility in Grenoble, France. His talk on "New Perspectives" covered both problems and strategies which are faced in a powder diffraction experiment at a synchrotron source.

Prof. A. F. Witt, Massachusetts Institute of Technology, Cambridge, MA, USA, and Prof. Priesinger presented the basic ideas in a planned project called "EURO-CRYST: An Austrian Initiative for European Collaboration in Crystal Growth Research and Technology". EURO-CRYST is aimed to be the first center of excellence for long-range collaborative European research in science and technology of crystal growth and characterization, which will be located in Austria.

The Poster sessions comprised 200 contributions distributed over three afternoons. For each session a "most informative and best looking poster" was designated.

The meeting was a success for Professor Priesinger and his coworkers in the organizing committee. We look forward to EPDIC-4, to be held in Chester, UK in 1995.

R. J. Cernik

Southern Africa Powder Diffraction Workshop PDSA-94

An International Workshop on Advanced Powder Diffraction Techniques in Mineral and Materials Processing will be held at the South Africa Geological Survey in Pretoria, South Africa, 24-27 October 1994. It is organised by the South African Crystallographic Society and the Mineralogical Association of South Africa in collaboration with the Commission on Powder Diffraction of the IUCr.

Special emphasis will be given to applications in the analysis of ores and modern solid state materials. The workshop will be followed by a number of optional short excursions to mineralogically important sites or industries that employ X-ray techniques. Morning and afternoon lectures (invited) will be followed by tutorials and demonstrations. Poster sessions with contributed papers by participants on their latest research findings, will be held in the evenings. Social events will include a traditional braai (outdoor barbecue). Numbers will be limited to 80 to keep the tutorial sessions small enough for personal attention.

For further information contact: Professor G. J. Kruger, Rand Afrikaans University, P O Box 524, Auckland Park 2006, Republic of South Africa. Tel: +27-11-489-2368; Fax: +27-11-489-2360; E-mail: **KRUGER@CHEMIE.RAU.AC.ZA.**

1996 IUCr SATELLITE MEETING ON POWDER DIFFRACTION

Plans are well under way to coordinate the 1996 IUCr Satellite Meeting on Powder Diffraction with the 45th Meeting of the Denver X-ray Conference. The dates for the meeting are planned for 3-8 August in Denver, Colorado, USA. The technical program and the local arrangements will be organized by representatives of both co-organizers.

There will be workshops and special sessions organized by each sponsor as well as many sessions and activities which will be of interest to all attendees. Details of this meeting will appear in the early circulars of the 1996 IUCr General Assembly and Congress to be held in Seattle, Washington, USA. Individuals interested in organizing workshops or special sessions at this meeting should contact one of the members of the CPD.

D. K. Smith

OPEN LETTER

Ab-initio solution of crystal structures via powder data: The role of a databank.

In the last 30 years, the phase problem for small crystal structures (based on single crystal data) has been practically solved. Even if the power and automation of Patterson methods was increased via a wide application of modern computer facilities, the primary credit should be ascribed to Direct Methods. More sound probabilistic approaches and new algorithms today allow the automatic solution of up to say 100-150 atoms in the asymmetric unit even when no heavy atom is present.

The free circulation of the experimental data has been a non-negligible factor in the tremendous success of Direct Methods. Data of structures difficult to solve constitute valid tests for the various direct approaches and often are the occasion for the formulation of new theories. A small data bank of about 40 "difficult" crystal structures has been compiled and distributed by George Sheldrick which proved very useful.

When only powder data are available, crystal structure solution is still a difficult job even for small molecules. Casual or systematic reflection overlapping, preferred orientation, background estimation and several other geometrical and physical factors make uncertain the phasing process, and the structure solution often remains difficult.

The challenge over the next few years is to make the crystal structure solution routine even from powder data. My personal experience with crystal data suggests that the free circulation of powder data could play a central role for the advancement of crystal structure solution methods. I propose

through this letter the constitution of a data bank including structures "difficult" to solve or solved in non-routine way.

The Bank should cover:

- a) data collected by synchrotron radiation, neutron and in-laboratory X-ray diffractometers, in order to face problems produced by different resolution of experimental devices and by the type of radiation (nuclear or electron scattering, imperfect monochromaticity, etc...);
- b) a variety of space groups, including those for which systematic overlapping of reflections occurs;
- c) a variety of experimental techniques (i.e., Bragg-Brentano, capillary, etc.) and a variety of detectors.

Any people wanting to contribute to such a bank should supply the complete intensity pattern collected at a fixed step of 2θ , complete information about the experimental techniques, space group, refined cell parameters, the atomic positions and thermal parameters, the structure resolution approach, and the references when available.

The intensity pattern rather than the IFI^2 set produced by a pattern decomposition program is preferable. Its availability could contribute to the advancement of the current techniques for pattern decomposition.

The bank should be available to any crystallographer upon request.

I hope CPD would actively support this proposal either by direct management or by entrusting it to another body.

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NEUTRON POWDER DIFFRACTION AT THE HIGH-FLUX ISOTOPE REACTOR OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TENNESSEE, USA

Recent developments in instrumentation at the High-Flux Isotope Reactor (HFIR) have brought on-line a high-resolution neutron powder diffractometer, which has been operating since 1991. The dedicated efforts of our technical and scientific team have brought this instrumentation from the conceptual design to a user-friendly and routinely-operating research tool. Upgrades to hardware and software are ongoing; however, this instrument has already demonstrated itself as an important addition to the expanding repertoire of experimental tools available at the HFIR.

Presently, the monochromator is a (115) Ge crystal, which can be oriented to select incident wavelengths of 1.0, 1.4, 2.2, and 4.2 Å. An array of 32 equally-spaced (2.7") ³He detectors, each with a similar foil Soller slit, can be step-scanned over a range of up to 40° for scattering angles between 11° and 135°2θ. Soller slits of 12' and 20' are positioned before and after the monochromator crystal, respectively. The design parameters give a resolution minimum of $\Delta d/d = 2 \times 10^{-3}$ at about 70° 2θ. A focusing Ge monochromator, which will provide greater intensity, is under construction and will be installed this year.

The diffractometer control program is user-friendly and operates presently on a VAX computer (running VMS), which is part of a network. A complete diffraction pattern can be obtained in a few hours depending upon the chosen 2θ range, step size and counting time. The status of the diffractometer can be checked remotely. An upgrade to the existing computer system and motor controllers is in progress and will significantly improve data collection times.

A variety of special environment devices are available to provide sample temperatures between 4.5 K and 1900 K. A clamp-type high-pressure cell can provide pressures up to 3 GPa. A selection of vanadium and aluminum cans are available, as well as the ability to spin or oscillate the sample to reduce preferred orientation effects. Sample volumes depend on the scattering power of the sample, but presently are in the range of 0.25 to 3 cm³. The high-pressure cell accommodates a 0.25 cm³ size

sample.

Local utility programs provide for instrumental calibration corrections, statistical check for noisy data points, individual detector displays, peak-fitting, pattern addition, pattern archiving and retrieval. A full range of software for Rietveld structure analysis (GSAS, RIETAN, LHPM), unit-cell refinement, and various crystallographic computations are also available.

Recent experiments performed on this instrument have included studies of the structures of the cuprate superconductors both under high pressure [1] and ambient pressure [2-3], phase transformations [4-5], crystal structure-property relationships in oxides [6-7] and structure refinements of other interesting oxides [8-9].

The HFIR is a user-facility and available for qualified experiments at no cost. Proprietary work can be done, but on a fee basis. As the new custodian of the HB4 powder diffractometer, I invite you to consider the use of neutron powder diffraction at the HFIR. Contact me with your questions and proposals.

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NEWS FROM ICDD

In December 1993, the International Centre for Diffraction Data announced the awarding of three Crystallography Scholar-

ships for 1994. The recipients were: Peter C. Burns, The University of Manitoba, Canada; Annapoorna Akella, Oregon State University, USA; and Michael Lloyd, University of Kentucky, USA. Peter Burns is conducting graduate studies on the stereochemistry of Cu^{2+} oxysalt minerals. Annapoorna Akella is identifying important correlations between atomic structure and luminescent and nonlinear optical properties. Michael Lloyd is researching the probability of the formation of solid state compounds.

The Board of Directors of the International Centre for Diffraction Data designated Dr. Larry D. Calvert and Prof. Yoshio Takeuchi as Distinguished Fellows of ICDD for their sustained outstanding contribution to the organization and in the field powder diffraction. Since 1982, eleven members have been elected as Distinguished Fellows. Dr. Calvert is the first ICDD member to receive this honor posthumously.

At the October 1993 meetings of ICDD, the new facilities were dedicated with



the Official ribbon cutting ceremony. The duties were carried out by the Distinguished Fellows of ICDD. Participating in the Ceremony along with ICDD Chairman Gerald G. Johnson, Jr. (in the sweater in the photograph on the previous page) were, left to right: Ben Post, Mary E. Mrose, Sigmund Weismann, Ludo K. Frevel, and Howard F. McMurdie. The photograph was taken at the Official moment. Distinguished Fellows, Jesse W. Caum and Arthur J. C. Wilson were unable to attend.

Results of the 1994 election for the Board of Directors are:

Chairman: Gerald G. Johnson, Jr.
 Vice Chairman: Helein D. Hitchcock
 Chairman, Technical Committee:
 Ting C. Huang
 Members at Large: Thomas N. Blanton
 Cyrus E. Crowder
 Charlotte Lowe-Ma

Continuing members of the Board of Directors are:

Past Chairman: Ludo K. Frevel
 Members at Large: Melvin H. Mueller
 Walter Eysel
 Treasurer: Gerhard R. Fischer

New products of interest to powder diffractionists are the MINERAL POWDER DIFFRACTION FILE, DATA BOOK and SEARCH MANUAL and the revised publication of SETS 14-15 DATABOOK. The MINERALS POWDER DIFFRACTION FILE DATABOOK and SEARCH MANUAL contain more than 3800 patterns representing 3200 minerals. The data contained in the SETS 14-15 DATABOOK were first published in databook form in 1972. The data contained in the new publication have been through an extensive editorial review and evaluation process. Additional information about ICDD products may be obtained by calling +1-610-325-9810.

Ludo Frevel
 ICDD Representative

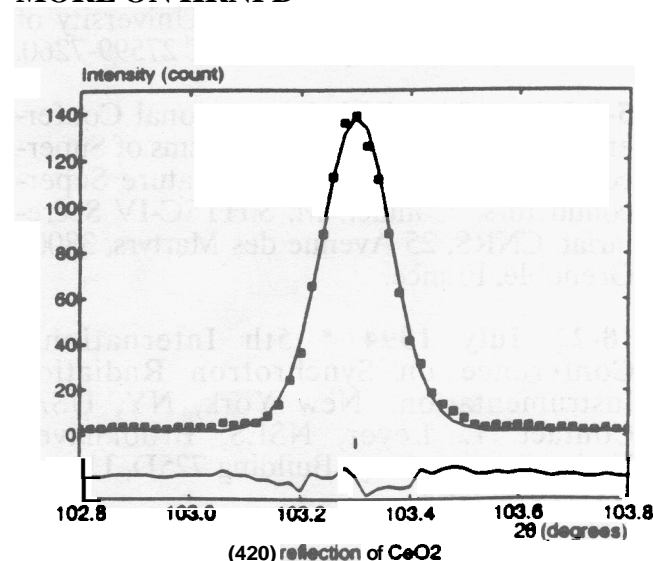
ANNOUNCEMENT OF THE ICDD 1995 CRYSTALLOGRAPHY SCHOLARSHIPS

Applications for the 1995 ICDD Scholarship awards are now being accepted. The applicant should be a graduate student seeking a degree with a major interest in crystallography (crystal structure analysis, systematic classification of crystal structures, crystal morphology, modulated structures, correlation of atomic structure with physical properties, phase identification and materials characterization). There are no restrictions on country, race, age or sex. The term of the scholarship is one year with the possibility of a one year renewal. The \$2000 awards will be on a competitive basis considering all the applications received up to the closing date.

Scholarship applications should contain a Curriculum Vita, a one page proposal describing the type of crystallographic research to be partially supported by the scholarship and a supportive letter from the sponsoring professor of an accredited university or an institute of technology.

Applications should be submitted by 31 October 1994 to: Secretary, International Centre for Diffraction Data, Newton Square Corporate Campus, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. Further information on this award may be obtained from the same address.

MORE ON HRNPD



Example of peak shapes obtained from the HRNPD installation at Brookhaven National Laboratory (See article on HRNPD in Newsletter 11)

FUTURE MEETINGS

14 June 1994 * British Crystallography Group Meeting on Public Domain Software for X-ray Powder Diffraction Studies. SERC, Daresbury Laboratory, Cheshire, UK. Contact: Dr. D. J. Dyson, British Steel Technical, Swinden Laboratories, Moorgate, Rotherham, South Yorkshire S60 3AR, UK.

19-23 June 1994 * International Conference on "Powder Diffraction and Crystal Chemistry". St. -Petersburg, Russia (the "white nights" period), on the base of St. -Petersburg University in Peterhof, a suburb of St. -Petersburg. The scientific programme is being coordinated by the Commission on Powder Diffraction. It will include invited lectures, other oral presentations and poster sessions. The official language of the Conference will be English. Applications for participation in the Conference should be sent to the Organizing Committee as early as possible. Committee Chairman: Prof. S. K. Filatov, Department of Crystallography, St. -Petersburg University, University Embassy, 7/9, St. -Petersburg, 199034, Russia. Tel: (812) 2189-647; FAX: (812) 2181-346, E-mail: FLT@DEAN.GEOLL.SPB.SU.

26 June- 1 July 1994 * American Crystallographic Association, Atlanta, Georgia. Contacts: Loren Williams, Local Chairman, Department of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332 and Charles Carter, Program Chairman, Department of Biochemistry and Biophysics, University of North Carolina, Chapel Hill, NC 27599-7260.

5-9 July 1994 * IVth International Conference on Materials and Mechanisms of Superconductivity and High-Temperature Superconductors. Contact: M. S.HTSC-IV Secretariat, CNRS, 25 Avenue des Martyrs, 38000 Grenoble, France.

18-22 July 1994 * 5th International Conference on Synchrotron Radiation Instrumentation. New York, NY, USA. Contact: L. Lever, NSLS, Brookhaven National Laboratory, Building 725D, Upton, NY 11973, USA.

2-6 August 1994 * Annual Denver X-ray Conference. Denver, Colorado. Contact: Prof. Paul K. Predecki, Department of Engineering, University of Denver, Denver, CO 80208, USA. FAX: +1-303-871-4450; E-mail: DENXRCON@DIANA.CAIR.DU

.EDU.

22-26 August 1994 * XVI CAC, XVI Conference on Applied Crystallography. Cieszyn, Poland. Chairman: Prof. H. Morawiec, University of Silesia. Contact: Dr. D. Stroz, Institute of Physics and Chemistry of Metals, University of Silesia, Bankowa 12, 40-007 Katowice, Poland. Tel: +4832-596929; FAX: +4832-599605; E-mail: DANA@USCTOUXI.CTO.US.EDU.PL.

21-26 August 1994 * Tenth International Conference on the Strength of Materials. Sendai, Japan. Contact: ICSMA-10, c/o Dr. K. Maruyama, Department of Materials Science, Faculty of Engineering, Tohoku University, Sendai 980, Japan.

28 August- 2 September 1994 * ECH-15, 15th European Crystallographic Meeting. Dresden, Germany. Contact: Prof. P. Paufler, Institut für Kristallographie, Fachbereich Physik, Technische Universität Dresden, Mommsenstrasse 13, D-0-8027 Dresden, Germany. Tel: +37-3-51-463-3378; FAX: +37-3-51-463-7109.

4-9 September 1994 * 16th General Meeting of the International Mineralogical Association. Pisa, Italy. Contact: Dr. . Merlino, Chairman IMA 94, Dipartimento di Scienze della Terra, Università di Pisa, Via S. Maria 53, I-56126 Pisa, ITALY. FAX: +39-50-40976; E-mail: IMA94@VM.CNUCE.CNR.IT.

3-7 October 1994 * Conference on Applied Crystallography. Liptovsky Mikulas, Slovakia. Contact: Dr. J. Fiala, Department of Metallurgy, Central Research Institute SKODA, Tylova 46, 31600 Pizen, Czech Republic. FAX: +42-19-220-762.

5-7 October 1994 * International Seminar on Neutron Scattering at High Pressure. Dubna, Russia. Contact: Dr. B. N. Savenko, Frank Laboratory for Neutron Physics, Joint Institute for Nuclear Research, 141980 Dubna, Moscow region, Russia. Tel: +7-096-21-62498 or +7-095-92-43914; FAX: +7-096-21-65085; E-mail: SAVENKO@NFSUN1JINR.DUBNA.SU.

11-14 October 1994 * International Centre for Diffraction Data Fall meeting. Newtown Square, Pennsylvania, USA. Contact: Mr. J. Messick, ICDD, 12 Campus Boulevard, Newtown Square, PA 19073, USA. FAX:

+1-610-325-9823; E-mail: MES-SICK@ICDD.COM.

24-27 October 1994 * PDSA-94 - The International Workshop on Advanced Powder Diffraction Techniques in Minerals and Materials Processing. Geological Survey of South Africa, Pretoria, South Africa. Contact: Prof. G. J. Kruger, Rand Afrikaans University, P. O. Box 524, Auckland Park 2006, Republic of South Africa. Tel: +427-11-489-2368; FAX: +427-11-489-2360; E-mail: KRUGER@CHEMIE.RAU.AC.ZA.

17-19 November 1994 * Crystallographic Society of Japan Annual Meeting. Osaka, Japan. Contact: Prof. Yukiteru Katsube, Osaka University, Osaka, Japan. Tel: +81-6-877-5111; FAX: +81-6-874-2533.

10-15 July 1995 * EPDIC-IV. Chester College, UK. Contact: Dr. R. J. Cernik, SERC, Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK. FAX: +44-0250603-174 or 100; E-mail: CER-NIK@DARSBURY.AC.UK.

16-20 July 1995 * Ab-Initio Structure Determination Using Powder Diffraction Techniques. Oxford, UK. Contact: Dr. W. I. F. David. E-mail: WIFD@ISISE.RL.AC.UK.

23-28 July 1995 * American Crystallographic Association Meeting. Montreal, Quebec, Canada. Contact: Dr. Y. LePage, Program Chairman, NRC of Canada, Chemistry Department, Ottawa, Ontario, K1A 0R6, Canada. Tel: +1-613-993-2527; FAX: +1-613-952-1275; E-mail:

YVON@IECEMS.LAN.NRC.CA. Local Chair: Dr. M. Cygler, Biotechnology Research Institute, 6100 Royalmount Avenue, Montreal, Quebec PQ H4P 2R2, Canada. Tel: +1-514-496-6321.

6-11 August 1995 * 16th European Crystallographic Meeting. Lund, Sweden. Contact: Dr. Ake Oskarsson (Chairman). Department of Inorganic Chemistry 1, Chemical Center, Lund University, P. O. Box 124, S-221 00 Lund, Sweden. Tel: +46-46-108102; E-mail: AKE.OSKARSSON@INORGK1.LU.SE.

21-25 August 1995 * International Conference on X-ray Powder Diffraction Analysis of Size/Strain, Macrostress, and Texture. Liptovsky Mikulas, Slovakia. Contact: Dr. J. Fiala, Department of Metallurgy, Central Research Institute SKODA, Tylova 46, 31600 Pizen, Czech Republic. FAX: 1+42-19-220-762.

3-9 August 1996 * Satellite Meeting on Powder Diffraction associated with the IUCr Congress on Crystallography and Denver X-ray Conference. Denver, Colorado. Contact: Prof. Paul K. Predecki, Department of Engineering, University of Denver, Denver, CO 80208, USA. FAX: +1-303-871-4450; E-mail: DENXCON@DIANA.CAIR.DU.EDU.

8-17 August 1996 * 17th IUCr General Assembly and International Congress of Crystallography. Seattle, Washington, USA. Contact: Prof. R. F. Bryan, Department of Chemistry, University of Virginia, Charlottesville, VA 22903, USA.

MAILING LIST FOR NEWSLETTERS

For those persons who did not receive a personal copy of this issue of the Newsletter and who would like to receive a personal copy of future issues, please make sure that your name is on our mailing list by completing a copy of this form and mailing it to the CPD Secretary, Dr. Daniel Louër at his address shown below. You may also use this form to notify us of a change of address, or to let us know of anyone else who might like to receive the Newsletter.

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Please mail the completed form to Dr. Daniel Louër, Laboratoire de Cristallochimie, Chimie Solide et Inorganique Molecule, Université de Rennes I, 35042 Rennes, Cedex, France.

CALL FOR CONTRIBUTIONS TO THE NEXT CPD NEWSLETTER

The next issue of the CPD Newsletter will be edited by Dr. R. J. Cernik to appear in October of 1994. He would greatly appreciate contributions from readers on matters of interest to the powder diffraction community, e.g. meeting reports, future meetings, developments in instruments, techniques, and computer programs and news of general interest. Please send articles and suggestions directly to him at: SERC, Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK.

D. K. Smith, Editor of CPD-NL12

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