

COMMISSION ON POWDER DIFFRACTION

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

NEWSLETTER No. 11, NOVEMBER 1993

THE ICDD MOVES FORWARD

In the 1940's, with support from the Dow Chemical Company, the General Electric Company, the Pennsylvania State University, the American Crystallographic Association, the Institute of Physics (British), the National Bureau of Standards, and the American Society for Testing and Materials (ASTM), the "Joint Committee on Chemical Analysis by X-ray Diffraction Methods" published a collection of 1,000 data cards of X-ray powder diffraction patterns. The first publication of diffraction patterns was composed largely of data from the Dow Chemical Company collection. The importance of this information to science and industry was immediately recognized. Today, this collection has increased to over 60,000 well-characterized numerical representations of X-ray diffraction patterns. It is known throughout the world as the Powder Diffraction File. The patterns included in the Powder Diffraction File are generally accepted as the standards for X-ray diffraction analysis.

As the Powder Diffraction File grew and matured, so did the organization that created it. In 1969, the ASTM Joint Committee on Chemical Analysis by X-ray Diffraction Methods incorporated as the Joint Committee on Powder Diffraction Standards. Today, it is known as the International Centre for Diffraction Data (ICDD). Readers of this newsletter may be interested to know that the ICDD has been a Scientific Associate of the IUCr since 1987.

The ICDD mission is to collect, edit, publish and distribute to the public, data in suitable form to serve as reference standards within the area of materials

characterization, and to sponsor suitable research projects for the improvement, development and utilization of data for such purposes. To accomplish this goal, the following organizations cooperate with ICDD's dedicated volunteer scientists:

- American Ceramic Society
- American Crystallographic Association
- American Society for Testing and Materials
- Australian X-ray Analytical Association
- British Crystallographic Association
- The Clay Minerals Society
- Deutsche Gesellschaft für Kristallographie
- Deutsche Mineralogische Gesellschaft
- The Institute of Physics
- The Mineralogical Association of Canada
- The Mineralogical Society of America
- Mineralogical Society of Great Britain and Ireland
- Société Française de Mineralogie et de Crystallographie

ICDD's first headquarters was located in a single room in a rented house on Heister Street in State College, Pennsylvania. During the 1950's and 1960's the Powder Diffraction File was published from the ASTM Building in Philadelphia. ASTM served as the headquarters location until the Centre incorporated in 1969. The Centre moved to its temporary headquarters on Rittenhouse Square in Philadelphia in 1970. Early in 1971, the Centre relocated to 1601 Park Lane, Swarthmore, Pennsylvania where it established its permanent headquarters. Today, the



ICDD Headquarters, Newtown Square, Pennsylvania

International Centre is proud to announce the relocation of its new international headquarters to Newtown Square, Pennsylvania.

The decision to construct a new headquarters facility was made after careful consideration and deliberation by two recent Boards of Directors. During the late 1980's and early 1990's it became apparent that if the ICDD were to satisfactorily meet the growing demands created by the increasing international distribution of its products, the continuing demand to supply the most accurate up-to-date information and search procedures available, and to increase its educational and instructional programs to meet the needs of new diffractionists, the Centre itself had to provide room for growth. It became apparent that the ICDD's mission could not be accomplished in the existing facility in Swarthmore.

The new headquarters - a striking brick and glass one story building of 25,000 square feet - is situated on a 6.5 acre site located in the Newtown Square Corporate Campus in suburban Newtown Square, Pennsylvania - about 17 miles northwest of the Philadelphia International Airport.

Each section of the building has been designed to accommodate specific functions. The operational section provides for the administrative, computer, financial, business, grants/education, journal, sales/marketing, editorial, production and warehousing operations. Included in this section are twenty-seven individual offices for the professional and management staff, an area dedicated to editorial/production operations, a Sales Department that includes five work stations, a well-designed five hundred square foot computer facility, a small library and individual file rooms for each operating department. Work rooms have been provided for the Powder Diffraction journal operations and grant/education activity.

The conference section of the building was designed to support the International Centre's meetings and educational activities. This wing provides a facility where the ICDD's volunteer members can meet and rooms adequately equipped to conduct educational programs, seminars and the ICDD XRD and XRF clinics.

The International Centre has grown over the years from a group of only three individuals working in a single small room, to a volunteer membership of more than 100 scientists and a staff of 30 highly skilled individuals operating out of a spacious modern facility. Contributing to the success and growth of the ICDD have been the scientific contributions by the Centre's membership to enhance the Powder Diffraction File and an enthusiastic research and development program that has kept the Centre abreast of modern day technology.

Presently the International Centre is developing methods to streamline its editorial process to provide for more rapid, accurate and cost-effective entry of data; state of the art CD-ROM development to enhance its most popular product; the use of video for education and training in areas such as search-match procedures, diffractometer alignment, and the use of computer software; the publishing of a data base containing full diffraction patterns for materials such as clays and polymers and the presentation of ancillary X-ray diffraction references on CD-ROM. These projects, coupled with the International Centre's Grant-in-Aid program to develop and improve the utilization of the

Powder Diffraction File, present tomorrow's solutions to today's challenges. The Centre accepts these challenges, embarking on an era that will provide for even more growth than experienced in the past.

The members and staff of the International Centre are proud of their new facility and extend to all interested diffractionists an invitation to visit the headquarters when in the Greater Philadelphia area.

Gerald G. Johnson, Jr.
Chairman
International Centre

Julian Messick
Corporate Secretary
International Centre

RUSSIAN ASSOCIATION "POWDER CRYSTALLOGRAPHY" FOUNDED

Russian Association "Powder Crystallography" was founded in January 29, 1993 in the Chernogolovka Moscow region at a general meeting of about 100 participants from approximately 25 universities, scientific societies, Institutes of the Russian Academy of Science and some other organizations. The Association "Powder Crystallography" is a non-governmental and non-profit organization of researchers who specialize mostly in the field of the investigation of natural and synthetic materials by diffraction methods. The Association was supported by the National Crystallographic Committee of Russia (Academician B. K. Vainshtein) and by scientific organizations such as the Moscow State University, Institute of Solid State Physics (Chernogolovka, Moscow region), Institute of Crystallography (Moscow), Research Institute of Physical Chemistry (Moscow), Institute of Chemistry of Silicates (St. Petersburg), Institute of Catalysis (Novosibirsk) and others.

The directions of future activity of the Association include: the development of hardware, software, and data bases; mineralogy; chemistry and materials science; neutron diffraction; electron diffraction; structure analysis; theoretical aspects of powder crystallography; education, etc. An important task of "Powder Crystallography" is the unification of the efforts of researchers at universities, the Academy of Science and other scientific, educational, industrial and public organizations in Russia and abroad in the sphere of powder crystallography in order to create a developed informational area by issuing special literature and organizing conferences, seminars, and workshops devoted to the discussion of professional problems in powder crystallography. The Association will also enhance improvement of the existing experimental and theoretical basics of crystal structure determination as well as the creation of the most favorable conditions for full development of the intellectual potential of the members of the Association.

The location of the headquarters of the association "Powder Crystallography" is Moscow.

The president of the association is Prof. V. Sh. Shekhtman (Institute of Solid State Physics, Chernogolovka, Moscow region).

Vice Presidents: Prof. V. A. Dryts (Institute of Geology of Russian Academy of Science, Moscow); Prof. D. M. Kheiker (Institute of Crystallography of Russian Academy of Science, Moscow).

General Secretary: Dr. S. A. Ivanov (Research Institute of Physical Chemistry, Moscow).

Contact: Prof. V. Sh. Shekhtman, President of the Association "Powder Crystallography", Room 45, Building 2, Vavilov Street 44, Moscow - 333, 117333, Russia.

NEW HIGH RESOLUTION NEUTRON POWDER DIFFRACTOMETER (HRNPD) AT THE BROOKHAVEN HIGH FLUX BEAM REACTOR.

This new instrument offers resolution in neutron powder diffraction patterns exceeding that of many 'home laboratory' X-ray diffractometers in the angular region where the highest peak densities usually occur. First operated on 1 July 1993, the HRNPD has an instrumental profile which is smooth and nearly symmetric as well as narrow. Its minimum FWHM in the first weeks of operation was $\sim 0.15^\circ$ (2θ) (near 120°) with $11'-11'-5'$ collimators in place. This corresponds to $\Delta d/d$ in the 10^{-4} range. The unit features a 25-element 'Venetian blind' monochromator design and 64 ^3He detectors (see CPD Newsletter No. 7). With this unusually high resolution and an excellent flux-on-specimen (e.g., 3×10^5 n/cm² sec with the HFBR operating at half power), the HRNPD takes a leading place among the neutron powder diffractometers of the world. Many studies dependent on details of the reflection profiles (e.g., slight splitting from subtle phase changes, correct separation of the contributions from different phases, microstructure studies via details of 'line broadening') are made newly possible by it.

The HRNPD is to be operated as a national/international facility by a PRT (Participating Research Team) to which is allocated 50% of the instrument's time. The other 50% is available to general users, without charge for non-proprietary work, on a competing proposal basis. One may gain access to the instrument either as a general user or, on occasion, through collaboration with a PRT member. For a General User proposal form, write to Ms. Rae Greenberg, HFBR User Programs Administrator, Physics Department, Brookhaven National Laboratory, Upton, NY 11973 U.S.A. For a list of PRT members and their addresses, contact Prof. R. A. Young, PRT Chairman for the HRNPD, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332 U.S.A.

The CPD, 1987-1993

The IUCr Commission on Powder Diffraction (CPD) was established in August of 1987 by action of the IUCr General Assembly (GA) meeting in Perth, Australia. The initial members were Z. Bojarski (Poland), A. W. Hewat (France), R. J. Hill (Australia), J. I. Langford (United Kingdom, Secretary), P.-E. Werner (Sweden), T. Yamanaka (Japan) and R. A. Young (U.S.A., Chairman). The International Centre for Diffraction Data, being a Scientific Associate of the IUCr, appointed Ludo Frevel as their representative to the CPD. He serves as a de-facto member.

The members of the new Commission met 3 times during the Congress and identified the following as CPD projects to receive first consideration:

A computer-program (for analysis of powder diffraction data) exchange bank (later modified to a 'program information exchange bank' - 'PIXB')

A satellite meeting on powder diffraction for the Bordeaux Congress to be held in 1990 (SMP-90)

Sessions on powder diffraction at the Bordeaux Congress

An international workshop on Rietveld refinement to be held in May or June 1989

A CPD Newsletter to be issued twice yearly

A Round Robin survey of Rietveld refinement (RRRR) involving X-ray and neutron data and several samples

Generation of one or more new books on powder diffraction topics, e.g., the Rietveld method.

At the 1990 meeting of the GA, the original members were elected to new 3-year terms and 3 more members added: D. Louer (France, who had been program chairman for the SMP-90 and a consultant), D. E. Cox (U.S.A.), and J. Fiala (Czech Republic). As this commission has been very much a working commission with every member contributing something, all of the projects in the above list were established and several more were added. All have either been completed or are ongoing, as appropriate.

The PIXB and RRRR projects have each produced one publication and are now in phase 2. Ten newsletters have been issued, each edited by a different member of the CPD. The mailing list now numbers about 800 and 200-400 additional copies are distributed at powder-diffraction-related meetings. An International Workshop on the Rietveld Method was held at the ECN in Petten, The Netherlands, in June 1989. A multi-author book titled 'The Rietveld Method' was published by the Oxford University Press in April 1993.

The added projects include:

Four 3-day Summer Schools on the Rietveld Method (RSS) featuring hands-on experience in using the method on PC-type computers. Two were in Poland and one each in Argentina and Brazil (see below).

An inter-congress international meeting on powder diffraction, "Accuracy in Powder Diffraction II" held in May 1992 in the USA (at NIST, Gaithersburg, MD). The Proceedings were published in late 1992.

Co-organizers of the 'Fourth International Workshop of Crystallography. Computational Methods in X-ray Powder Diffraction Analysis' (PDSE-93) held in Aswan, Egypt in January 1993.

Development of the dictionaries needed and promotion of the general use of the CIF-STAR format for archiving and transferring of powder diffraction data. This is now a cooperative project with the ICDD.

A satellite meeting on powder diffraction (SMP-93) to be held in Hangzhou, P.R. China, 31 Aug. - 3 Sept. 1993 (see below).

A survey possibly leading to a Round Robin on determination of crystallite sizes and microstrain from powder diffraction data. This, also, is being done jointly with the ICDD.

It has been a pleasure and an honor for me to have been associated with such an active, cooperative, highly motivated and productive a group as is the Commission on Powder Diffraction.

I am also pleased to acknowledge the considerable

financial support the CPD has received from the IUCr for its various activities the cooperation of the ICDD including some direct financial support for RW-89, SMP-90, APD-II, PDSE-93. and SMP-93.

R. A. Young, Chairman 1987-93
CPD of the IUCr

Outcomes from the Business Meetings of the CPD held during the XVth IUCr Congress and PD Satellite in China

The Commission on Powder Diffraction held two Business Meetings during the Beijing Congress and the Hangzhou Satellite Meeting on Advances in Powder Diffraction. The outgoing Chairman, Prof. R. A. Young (USA), and the incoming Chairman, Dr. H. J. Hill (Australia), were also present at an IUCr Executive Committee meeting in order to present the report of the CPD for the 1990-93 triennium, and to propose the CPD budget and membership nominations for 1993-96.

The major points of discussion and outcomes from these meetings were as follows:

- The nominations for membership of the CPD for 1993-96 were:

- Dr. R. J. Hill, Australia (Chairman)

- Dr. R. J. Cernik, UK

- Dr. D. F. Cox, USA

- Dr. J. Fiala, Czech Republic

- Prof. Shao-Fan Lin, PR China

- Dr. D. Louer, France

- Dr. L. B. McCusker, Switzerland

- Prof. D. K. Smith, USA

- Dr. I. G. Tellgren, Sweden

- Dr. H. Toraya, Japan

- Dr. L. Frevel, USA (ICDD-JCPDS representative)

- These nominees were accepted by the EC and were subsequently elected unanimously by the General Assembly.

- The EC has provided support for the CPD to continue to prepare and circulate its own Newsletter throughout the next triennium. As previously, extracts from the CPD Newsletter will be included in the IUCr Newsletter as required.

- CPD Newsletter No 10 is being translated into Chinese through the good auspices of Prof. Lin of the CPD. About 300 copies will be distributed with a Chinese version of the journal Powder Diffraction in October/November, 1993.

- Plans for CPD sanctioned and/or organized meetings over the next triennium include:

- St. Petersburg, Russia, in June 1994

- Pretoria, South Africa, in October 1994

- Oxford, UK, in July 1995

- Liptovsky Mikulos, Slovakia, in September 1995

- Denver, USA, in September 1996

R. J. Hill

MEETING REPORTS

ADVANCES IN POWDER DIFFRACTION-SMP-93

Hangzhou, China, 31 August - 3 September 1993

A Satellite Meeting of the IUCr XVth Congress & General Assembly

A major activity of the Commission on Powder Diffraction during the past triennium has been the organization of the Powder Diffraction Satellite Meeting, held in Hangzhou immediately after the IUCr Beijing Congress. The main aim was to present recent developments in powder diffraction theory and practice and to emphasize the power of modern diffraction methods in materials science. The resulting scientific programme certainly appealed to the powder diffraction community, since the meeting attracted about 140 registrants with a diversity of interests and from 18 different countries.

The meeting was held in the luxurious Shangri-La Hotel, surrounded by mountains and overlooking the islands, causeways and bridges of the West Lake at Hangzhou. This is said, with some justification, to be one of the most beautiful regions of China. The participants were welcomed by Mr. Zhan Shao-Wen, representing the Zhejiang province. Prof. Ling Rong-Guo, Chairman of the Organizing Committee, Prof. Shen Shan-Hong, President of Hangzhou University, and Dr. Rod Hill, Chairman of the CPD. Prof. Tao Kun then gave the opening address, on X-ray powder diffraction in China, and the remainder of the first day was devoted to structural studies from powder data, theory and techniques in the morning and applications in the afternoon. The first invited lecture, on maximum entropy and likelihood estimation, was given by Dr. Chris Gilmore and this was followed by a talk by Prof. Carmelo Giacobozzo on direct methods. The session on applications was introduced by Dr. Andy Finch (combined neutron and synchrotron X-ray studies) and Dr. Michael Estermann (ab initio structure solution of zeolites). During this session Dr. Rod Hill reported on the outcome of the CPD Round Robin on Rietveld Refinement. Instrumentation, standards and databases were the topics covered during the morning of the second day. Dr. Ron Jenkins opened this session with a lecture on new developments in PC-based data retrieval programs and Dr. Malcolm McMahon reviewed the use of image-plate detectors in powder diffraction. The important topics of non-ambient and time-dependent experiments were covered during the afternoon, the speakers being Prof. Y. Fujii (advances in synchrotron X-ray powder diffraction under high pressure) and Prof. Takamitsu Yamanaka (application of time-resolved diffraction to the study of structural transitions and solid-state reactions). The use of powder diffraction in studying microstructure and other characteristics of materials was the theme of the final session, during the morning of 3 September. The opening invited lecture was given by Prof. Hans Bunge on the effects of texture in powder diffraction and Prof. Wang Yu-Ming then spoke on the correlation between microstructure and mechanical behaviour. In addition to the invited lectures, there were 25 oral contributions, selected from the submitted abstracts, and 86 posters.

In addition to the main scientific programme,

complementary workshops were arranged by the International Centre for Diffraction Data. These were conducted by Dr. Ron Jenkins, assisted by Drs. Ting Huang and Fang-Ling Needham and Prof. Walter Eysel, and were well attended.

The undoubted success of the entire meeting was due in no small measure to the hard work of Prof. Ling Rong-Guo and his team over a long period and to sustained effort on the part of the Programme Committee. Such meetings could not take place without a substantial commitment in terms of local manpower and resources and these were freely made available by Hangzhou University. A copy of the 146-page book of abstracts can be obtained, at a cost of \$20, from Prof. Ling Rong-Guo of the Central Laboratory, Hangzhou University, Hangzhou, China.

J. Ian Langford, Chairman, Programme Committee

Powder Diffracton at the XVth IUCr Congress

Powder diffracton was very strongly represented at the Beijing Congress of the IUCr. Two Microsymposia, two Poster Sessions, two Discussion Sessions and a Workshop were devoted exclusively, or nearly exclusively, to powder diffraction. In addition, powder diffraction was featured in several other microsymposia and poster sessions, where it was the tool of choice for obtaining many important new scientific results.

Areas in which the study of powdered materials were particularly evident, and crucial to the progress made, were those dealing with fullerenes, zeolites, and high temperature superconductors.

The Microsymposium and Poster Session on Strategies for ab initio Structure Determination from Powder Data (Chairperson, C. Gilmore and L. D. Ma) clearly showed that this is a very popular and rapidly emerging field which should yield many exciting outcomes over the next few years. A wide range of techniques and software are now being used to assist the solution of crystal structures from powder data collected in the laboratory, as well as at major synchrotron X-ray and neutron facilities. These techniques include the more traditional direct methods common to single crystal work, together with the emerging powerful techniques of entropy and likelihood maximisation, with or without the use of prior chemical knowledge. The precision and accuracy of the results obtained for several materials are such that the subtle details of their electron density distributions and thermal vibration parameters have now been reported.

The Microsymposium on X-ray and Neutron Powder Diffracton (Chairpersons, A. W. Hewat and C. L. Guo) provided some spectacular examples of the power of computer-based structure modelling as a complement to diffraction studies, and also of the potential for the combined use of X-ray and neutron data to provide solutions to very difficult structural problems.

The Discussion Session on Multiphase Analysis (Chairpersons, T. C. Huang and Y. M. Wang) provided a timely update on progress with search/match procedures using the full diffraction pattern collected from multiphase mixtures. Other presentations related to the current status

and recent developments in quantitative phase analysis using the Rietveld and two-stage methods. All of the papers made it clear that the use of the full profile provides many advantages over the traditional integrated intensity techniques for both identification and qualification. This is now being recognized by the ICDD-JCPDS through its decision to store the full powder diffraction pattern in the PDF-3 database.

The Discussion Session on High Pressure Techniques for Crystallography (Chairperson, H. Schulz) provided some recent exciting developments in the instrumentation for high pressure powder diffraction using X-rays and neutrons and pointed to an imminent substantial increase in the pressures that will soon be accessible for the study of polycrystalline materials. Prospects for simultaneous high temperature and pressure work are also good.

The large number of papers at the Congress dealing with novel software, hardware and technique developments in powder diffraction, the breadth of topics and materials covered, and the high level of activity and interest are evidence that powder diffraction is no longer (if it ever was) merely an interesting side issue in crystallography. It is now firmly entrenched as part of the mainstream.

R. J. Hill and R. A. Young

EPDIC-3

The Third European Powder Diffraction Conference was held on 25-28 September, 1993, at the Technical University of Vienna. Some 340 diffractionists from 26 different countries attended a well organized and scientifically stimulating meeting. Six invited lecturers covered the following topics:

R. L. McGreevy: Structural disorder: what you can learn from diffuse scattering by reverse Monte Carlo modelling.

H. E. Göbel: Grazing incidence powder diffraction and reflectometry - a powerful combination for non-destructive thin film analysis.

F. Bouree: Neutron powder diffraction and magnetic structures.

T. Ungár: Characteristically asymmetric X-ray line broadening, an indication of microscopic residual stresses.

M. I. McMahon and R. J. Nelmes: Angle-dispersive powder diffraction at high pressure.

P. Suortti: Powder diffraction with synchrotron radiation: new perspectives.

The main lectures were followed by 20-minute oral presentations in the morning and poster sessions in the afternoon. Nine different topics were addressed, with the (number) of papers/posters shown:

1. Diffraction under non-ambient conditions (29)
2. Characterization of thin films (14)
3. Structures and phase transitions of magnetic materials (10)
4. Amorphous and disordered material (14)
5. Qualitative and quantitative phase analysis (25)
6. Stress, texture, and crystallite size analysis (18)

7. Crystal structure determination from powder diffraction data (39)
8. New instrumentation and experimental methods (16)
9. Advances in diffraction software (14)

In addition, a commercial exhibition (comprising 13 manufacturers) took place in the entrance hall and on the first floor of the conference center. On Saturday, September 25, a workshop on the ICDD Powder Diffraction File was conducted by J. W. Visser and W. Eysel. A special feature of the conference was a feasibility study of the project EURO-CRYST (an Austrian Initiative for European Collaboration in Crystal Growth Research and Technology) presented by A. Preisinger and A. F. Witt.

L. K. Frevel

42nd Annual Denver X-Ray Conference August 2-6, 1993, Denver, Colorado

The 1993 Denver X-Ray Conference - 42nd in the series - was held August 2-6 in Denver, Colorado. The first 2 days were devoted to workshops, and the last 3 to oral and poster paper sessions on diffraction and fluorescence, as in past years. The Barrett Award for Diffraction was presented to Ron Jenkins of ICDD and was followed by the plenary session on "Impact of the PC in X-Ray Analysis", featuring papers by Jenkins (Historical Perspective), H. Goebel of Siemens (Future Aspects of PC-Controlled X-Ray Analysis), Q. Johnson of Materials Data Inc. (Software for XRD), and B. H. Toby of Air Products (Current and Future Developments in Desktop Computer Technology).

XRD or combined XRD/XRF special sessions were held on: Advances in Detectors, High-Volume X-ray Analysis, Synchrotron Applications, Stress Determination, Thin Film Applications, Full Pattern Analysis, Advances in Search/Match Methods, General Applications and Instrumentation. A total of 8 XRD-related or combined half-day workshops were presented on various topics. Attendance was 332 registered, with 36 companies exhibiting X-ray related products.

Paul K. Predecki

Rietveld Summer Schools and Workshops in South America, December 1992.

This report extends the brief account given in Newsletter No. 10. As was reported there, in cooperation with the local organizers the CPD organized Rietveld-method Summer Schools (RSS's) on 8-11 December 1992 at the National University of La Plata in Argentina and on 10-13 December at the University of Sao Paulo at Sao Paulo in Brazil. Student acquisition of individual 'hands-on' experience with running Rietveld refinements on PC-type computers was a principal objective of the RSS's.

Following the general scheme of the two previous RSS's organized by the CPD (August 1990 and 1992 in Poland) with the same professors (A. K. Cheetham, R. B. Von Dreele and R. A. Young) the program of the school consisted of lectures during the mornings, practical and tutorial sessions during the afternoons, and further

computer availability to students in the evenings. On the basis of their previous experience with the Rietveld method, the students were divided into two groups that rotated between practicals and tutorials. During practicals, two students (only) shared a computer and several advisors made themselves available. The fact that the programs used in the practicals were run on PC-type machines (286 with coprocessor at the minimum) made the experience especially relevant for the students, because computers of this sort are available in all South American laboratories.

The lectures were planned to lead the students smoothly from the foundations of powder diffraction to the latest applications of the Rietveld refinement and included valuable hints on matters like improvement of data collection, choosing the appropriate peak shape or dealing with non-structural contributions. The friendly atmosphere of the schools encouraged fluid scientific interactions between all the participants and allowed them to take full advantage of the tutorials and practical sessions.

The RSS in La Plata was followed by a day-long workshop on opportunities for establishing research collaborations. It consisted of a poster session followed by a general discussion on the applicability of Rietveld refinement to the topics investigated by the participants and then by personal interviews aimed at establishing research collaborations. The full value of this RSS and workshop will be known only in the future, but we can be certain that the main goals of the event have been achieved, i.e., the improvement of participants' skills in the use of Rietveld refinement and their introduction to new or combined techniques and/or alternative sources. In addition, the basis for scientific collaborations between lecturers and participants has been laid.

The last half-day the RSS in Sao Paulo was also the beginning session of the annual meeting of the Sociedade Brasileira de Cristalografia (SBCr). This provided opportunities for additional scientists to hear about Rietveld Refinement and the interests of the visiting professors in developing collaborative research projects. Besides the excellent educational opportunity offered by the school to the Brazilian crystallographic community, it also provided a useful occasion for the discussion of several current research projects in which the RR method could be applied. We foresee that in the future RR will be used by many of the participants and that fruitful collaborations will be initiated among several Brazilian research groups and also between some of the participants and the lecturers' research groups in the USA.

In Sao Paulo, the RSS was organized by the SBCr with the collaboration of a local committee formed by Y. P. Mascarenhas (chairperson), L. Q. do Amaral (president of the SBCr), M. C. A. Fantini and C. de O. Paiva Santos. In La Plata, the local organizing unit was the Continuous Studies Program of the Argentina National Diffraction Laboratory under the direction of Prof. Graciela Punte. In both cases, the local groups exerted much effort and attention to the taxing job of local organization and the results were excellent.

Financial support for some local expenses and travel grants for many of the students (only 30 - of 50 applicants from various South American countries - could be accommodated in the La Plata RSS and only 42 in Sao Paulo) was received from the CNPq, Philips Argentina S. A., and from the host institutions: the Molecular Physics Program of the Physics Department of the UNLP and the Physics Department of the University of Sao Paulo at Sao Paulo. The lecturers' trip expenses were supported by the U. S. National Science Foundation. Because that support was assured only at the last minute, underwriting of the travel of two lecturers by the IUCr's Visiting Professor program managed by the Commission on Teaching played a crucial role in allowing planning and scheduling of the event to proceed.

Prof. G. Punte and A. Goetta for the RSS in La Plata
Prof. Y. P. Mascarenhas for the RSS in Sao Paulo

FUTURE MEETINGS

November 4, 1993 - British Crystallographic Assn. 1993 ICG Autumn Meeting. Wrexham, UK. Contact: Dr. J. A. Jutson, Anal. Services, Wrexham Tech. Centre, BICC Cables Ltd., Wrexham, Clwyd, Wales LL13 9XP, UK.

March 28-31, 1994 - BCA Spring Meeting. Newcastle-Upon-Tyne, UK. Contact: Prof. W. Clegg, Dept. Chem., U. Newcastle, Newcastle-Upon-Tyne NE1 7RU, UK.

May 16-20, 1994 - Computational Methods in Chemical Design, Molecular Modeling - Theory and Experiment. Kloster Irsee near Kaufbeuren, Germany. Contact: Prof. C. Kruger, Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 4330 Mulheim a.d. Ruhr, Germany.

May 27-June 5 - 21st Crystallographic Course on Crystallography of Molecular Biology. Erice, Italy. Director: Wayne A. Hendrickson. Contact: L. Riva di Sanseverino, Dipto, Scienze Mineralogiche, Pza. Porta S. Donato 1, 40126 Bologna, Italy. FAX: 39 51 243336; e-mail: t54boml2@icineca.

June 19-23, 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 Organizing Committee as early as possible. Committee Chairman: Prof. S. K. Filatov, Dept. of Crystallography, St.-Petersburg University, University Emb., 719, St.-Petersburg, 199034, Russia. Phone: (812) 2189 647. FAX: (812) 2181 346. E-mail: FLTQDEAN.GEOLL.SPB.SU.

June 26-July 1, 1994 - American Crystallographic Association. Atlanta, Georgia. Contacts: Loren Williams, Local Chair, Dept. of Chem. and Biochem., Georgia Tech,

Atlanta, GA 30332 and Charles Carter, Program Chair, Dept. of Biochem. and Biophys., U. of North Carolina, Chapel Hill, NC 27599-7260.

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

July 11-15, 1994 - MacroAKRON'94 35th Int'l Symposium on Macromolecules. Akron, Ohio, USA. Contact: Cathy Manus-Gray, Symp. Coordinator, Inst. of Polymer Science, U. of Akron, Akron, OH 44355-3909 USA.

July 18-22, 1994 - 5th Int'l Conf. on Synchrotron Radiation Instrumentation. New York, NY. Contact: L. Lever, NSLS at Brookhaven Natl. Lab., Bldg. 725D, Upton, NY 11973, USA.

August 2-6, 1994 - Annual Denver X-ray Conference, Denver, Colorado. Contact: Prof. Paul Predecki, Dept. of Engineering, Univ. of Denver, Denver, CO 80208 U.S.A.

August 21-26, 1994 - Tenth Int'l Conf. on the Strength of Materials. Sendai, Japan. Contact: ICSMA-10, c/o Dr. K. Maruyama, Dept. of Matls. Sci., Faculty of Engrg., Tohoku U., Sendai 980, Japan.

August 23-27, 1994 - IXth Symposium on Organic Crystal Chemistry (OCC-94) which is a Satellite Meeting of ECM-15. Poznan, Poland. Program Chair: F. Herbststein, Israel Inst. of Technology. Contact: U. Rychlewska, Dept. of Chem., Adam Mickiewicz U., Grunwaldzka 6, 60-780 Poznan, Poland. e-mail: occ94@plpuamll.bitnet.

August 28-September 2, 1994 - ECM-I5, 15th European Crystallographic Meeting. Dresden, Germany. Contact: Prof. P. Paufler, Institut für Kristallographie, Fachbereich Physik, Technische U. Dresden, Mommsenstrasse 13, D-O-8027 Dresden, Germany. Tel.: 37 3 51 463 3378; FAX: 37 3 51 463 7109.

July 10-15, 1994 - EPDIC IV, Chester, U.K.

July 23-28, 1994 - ACA Meeting. Montreal, Canada. Contact: Y. LePage, Program Chair, NRC of Canada, Chem. Dept., Ottawa, Ontario K1A 0R6, Canada. Tel.: 613-993-2527; FAX: 613-952-1275; e-mail: yvon@ilan.nrc.ca. Local Chair: M. Cygler, Biotech. Res. inst., 6100 Royalmount Ave., Montreal, Quebec PQ H4P 2R2, Canada. Tel.: 514-496-6321.

August 6-11, 1995 - 16th European Crystallographic Meeting. Lund, Sweden. Contact: Ake Oskarsson (Chairman), Dept. of Inorganic Chem. 1, Chemical Center, Lund U., P. O. Box 124, S-221 00 Lund, Sweden. Tel.: 46 46 108102; e-mail: ake.oskarsson@inorgkl.lu.se.

August 8-17, 1996 - 17th IUCr General Assembly and Int'l Congress of Crystallography. Seattle, WA. Contact: Prof. R. F. Bryan, Dept. of Chem., U. of VA, Charlottesville, VA 22903 U.S.A.

MAILING LISTS 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 of this Newsletter, 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. R. J. Hill, 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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CALL FOR CONTRIBUTIONS TO THE CPD NEWSLETTER

The next issue of the CPD Newsletter will be edited by Prof. D. K. Smith to appear in the Spring 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: 239 Deike Bldg., The Pennsylvania State University, University Park, PA 16802, U.S.A.

Ludo Frevel, Editor of CPD-NII

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