

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President



The Executive Committee (EC) Meeting this year was held July 27-29 at Salt Lake City, USA, just after the ACA Meeting. All the EC members attended the meeting. Many important items were discussed at the meeting and some of these are described below. At the previous EC meeting held in Leuven, Belgium, it was approved (with the recommendation of the Finance Committee) that starting in 2008 *Acta Crystallographica* Section E should become an open-access journal. A number of discussion were held both within the Commission on Journals and the Finance Committee on how to reduce the workload for both editors and technical staff, and to keep the open-access submission fee as low as possible. As a result of these discussion a new short format for *Acta E* papers was introduced in 2007 and beginning in 2008 the submission fee for papers will be USD 150 for each paper accepted for publication. A waiver system will be introduced for submissions from developing countries.

As described in the previous issue, a PhD student from central Africa, Bernard Omondi, has successfully completed his PhD at the U. of Witwatersrand in South Africa, supported by an IUCr fund. The EC has approved continuation of this fund, but the system will be modified slightly: although the fund should be limited to a student from a sub-Saharan African country, the professor responsible for hosting the student and administering the fund may come from any country in Africa.

Next year, 2008, is the 60th anniversary of the formation of the IUCr in 1948. Several events are planned to celebrate this anniversary. The first is a Special Issue of *Acta Crystallographica* Section A, which will be published as the first issue of 2008. The second is an Anniversary Ceremony that will be held 23 August 2008 at Osaka, just before the Opening Ceremony of the 21st General Assembly and Congress. During the Anniversary Ceremony Ted Baker, a past President of the IUCr, will give a presentation on the central importance of crystallography to every facet of modern life. The third will be an exhibition of photographs. A variety of photographs from the past 60 years will be presented by Immediate Past President, Bill Duax, EC member Chris Gilmore and the first AsCA President, Syd Hall. Moreover, all past Presidents of the IUCr will be invited to participate in the Ceremony.

Details of the 21st General Assembly and Congress were reported by the Chair of the International Programme Committee, Yasuhiko Fujii. There will be 2 Plenary Lectures, 36 Keynote Lectures and 98 Microsymposia at the Congress. Approximately 1,500 poster presentations are expected with 500 posters to be presented every two days. Many official and optional tours to visit the neighbouring cities of Kyoto and Nara are planned. Details are given elsewhere in this issue (see pullout section between pages 12 and 13).

At the Leuven Meeting, the EC proposed that a number of non-member countries could form a group that would become a member of the IUCr. Discussions on potential groups were held during the council meetings of the three Regional Associates, ACA, AsCA and ECA. It is likely that at least one group will be formed in the region of each Regional Associate and the groups will be submitted for approval of their

membership at the next General Assembly in Osaka. This has the potential of adding more than 20 countries as new members of the IUCr. The EC will welcome these new members with pleasure. Nominations for the next President, Vice-President, General Secretary and Treasurer, and EC members made by the National Committees for Crystallography were considered by the Executive Committee. It was agreed that all the names received should be put forward for voting at the General Assembly at Osaka. This list has been sent to the National Committees. If the National Committees consider that other candidates should be put forward they are able to do so according to the By-Laws. I hope an active and effective EC will be elected by the General Assembly.

Yuji Ohashi, yohashi@spring8.or.jp

AWARDS AND PRIZES

American Crystallographic Association awards

The following awards will be presented at the ACA Annual Meeting in Knoxville, TN, USA, May 31-June 5, 2008.



Bi Cheng Wang

Bi Cheng Wang has been selected as the 2008 recipient of the A.L. Patterson Award for “significant contribution to the methodology of structure determination from single isomorphous replacement or single-wavelength anomalous scattering data and for its impact on structural biology.” This award is given to recognize and encourage outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information.



Radu Custelcean

Radu Custelcean (Oak Ridge National Lab, USA) has been selected to receive the 2008 Etter Early Career Award for “his creative research in crystal engineering of novel and functional metal organic framework structures for selective ion binding.” The award recognizes the outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career.

Call for nominations

2009 Bertram E. Warren Diffraction Physics Award

The American Crystallographic Assn (ACA) gives this award to recognize an important recent contribution to the physics of solids or liquids using X-ray, neutron, or electron diffraction techniques. Works published within a six-year period ending June 30 of the year preceding the award may be nominated. A monetary award of \$1,500, and up to \$1,500 travel expenses to accept the award at an annual meeting, and a certificate are awarded every third year. Established in 1970 by students and friends of Professor

Warren on the occasion of his retirement from the Massachusetts Inst. of Technology.

2009 Martin J. Buerger Award

This award is given to recognize mature scientists who have made contributions of exceptional distinction in areas of interest to the ACA. There are no restrictions as to nationality, race, sex, religion, or membership in the ACA. Awarded triennially in memory of Martin J. Buerger, Institute Professor Emeritus of M.I.T. and University Professor Emeritus of the U. of Connecticut, a mineralogist who made major contributions to many areas of crystallography. Established in 1983. The first award was made in 1985. Nominations for these awards are not limited to the USA and ACA membership is not a requirement.

Further information is available at www.amerocrystassn.com.

AWARDS AND PRIZES

Steitz receives Gairdner Award



Thomas A. Steitz

Yale biophysicist Thomas A. Steitz has received a 2007 Gairdner International Award for his groundbreaking work on the structure and function of the large subunit of the ribosome and the structural basis for the action of antibiotics that target the ribosome. Steitz established Rib-XPharmaceutical, Inc., which is using this knowledge of the structures of the large ribosomal subunit and its antibiotic complexes to create new classes of antibiotics.

NOTICE

BCA Industrial Group call for nominations

The British Crystallographic Assn Industrial group is giving an Industrial Crystallography Award to a UK crystallographers working in industry or in academic institutions. The award is given in recognition of a sustained contribution to industrial crystallography including crystallographic and diffraction work of all kinds.

Further information is available at img.cryst.bbk.ac.uk/BCA/IG/award/award.htm.

NOTICE

South African structural biology initiative

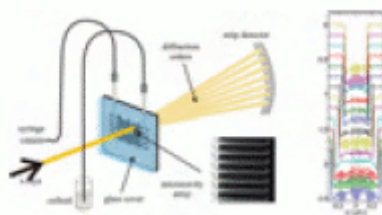
The aim of the South African Structural Biology Initiative is to firmly establish structural biology in Africa by exploiting the synergies that exist between the three universities in the Western Cape, the U. of Cape Town (UCT), the U. of the Western Cape (UWC) and the U. of Stellenbosch. UCT and UWC will jointly offer a Master's Degree in Structural Biology where highly regarded researchers in structural biology (X-ray crystallography, electron microscopy, nuclear magnetic resonance spectroscopy, computational modelling and bioinformatics) will collaborate to provide a world class teaching and research environment. The development of this program is funded by a generous grant from the Carnegie Corporation of New York. A unique feature of the Masters program is that students will have the opportunity of interacting with leading international experts in structural biology who will come to South Africa specifically to participate in the program. The establishment of structural biology as a formal discipline in South Africa will:

- Substantially increase local knowledge of biological structure
- Open the way to the determination of molecular structure locally
- Establish the manpower for industry based on structural knowledge, including structure based drug design.

IUCR JOURNALS NEWS

Diffractive imaging for periodic samples: retrieving one-dimensional concentration profiles across microfluidic channels

***Acta Cryst.* (2007). A63, 306-314 [doi:10.1107/S0108767307021903]**



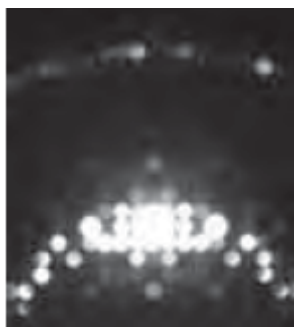
Left: Set-up to record X-ray small-angle scattering data for microfluidic arrays in transmission geometry. Right: The retrieved phase profiles across the channels reveal ordering effects in colloidal solutions. Geometrical confinement can dramatically alter bulk properties of fluids like viscosity and density and may be used for the alignment and, eventually, crystallization of macromolecules. We present a technique to determine the concentration profiles across microfluidic channels using iterative phase-retrieval algorithms applied to small-angle-grating diffraction data. Currently 300–600 nm sized channels are sampled with a resolution in the 10 nm range. We plan to scale the technique down further and to study otherwise non-crystallizable macromolecules.

O. Bunk, A. Diaz, F. Pfeiffer, C. David, B. Schmitt, D.K. Satapathy and J.F. van der Veen

IUCR JOURNALS NEWS

Chiral determination: direct interpretation of convergent-beam electron diffraction patterns using the series expansion of Cowley and Moodie

***Acta Cryst.* (2007). B63, 511-520 [doi:10.1107/S0108768107028595]**



A variety of methods, all involving multiple beam calculations, have been used for hand determination by convergent-beam electron diffraction. These are reviewed, along with the experimental and analytical requirements presented by differing point groups. It is found that, when a projected mirror line is present in a slightly tilted pattern, as shown, multiple beam calculations may be avoided and a simple formula involving structure factors can be used to determine the hand.

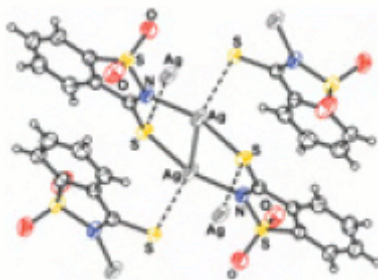
A.W.S. Johnson

IUCR JOURNALS NEWS

Poly[(μ_3 -1,1-dioxo-1,2-benzisothiazole-3-thiolato- κ^3 N:S3:S3)silver(I)]

Poly[(μ_3 -1,1-dioxo-1,2-benzisothiazole-3-thiolato- κ^3 N:S³:S³)silver(I)]

Acta Cryst. (2007). C63, m395-m397 [doi:10.1107/S0108270107035597]

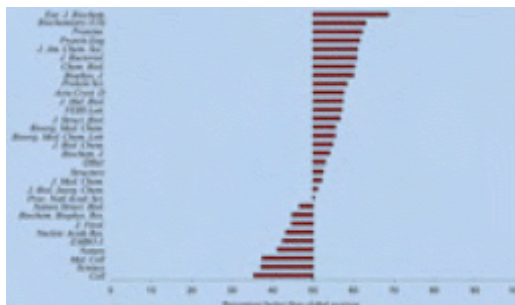


The crystal structure of the title compound $[\text{Ag}_2(\text{C}_7\text{H}_4\text{NO}_2\text{S}_2)_2]_n$ is described in this article. This new silver thiosaccharinate consists of dinuclear units in which two thiosaccharinate anions each bridge two silver atoms (by the endocyclic N and exocyclic S atoms) across a crystallographic center of inversion midway between the Ag atoms. The dimeric units are connected *via* $\text{Ag}-\text{S}_{\text{exo}}$ interactions to create two-dimensional networks. The Ag—Ag distance [2.9194(4)Å] can be considered a strong argentophilic interaction.

M. Dennehy, O.V. Quinzani and R.A. Burrow

Quality of protein crystal structures

Acta Cryst. (2007). D63, 941-950 [doi:10.1107/S0907444907033847]

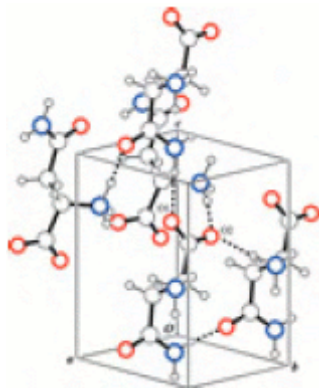


A method that will allow for comparison of crystallographic models deposited in the Protein Data Bank (PDB) (accounting for differences in resolution, protein size, sequence novelty and deposition date) has been developed. Analysis of structures reveals interesting features that indicate that the quality of deposited models in the PDB has not changed over time and the average quality of structures deposited by the structural genomics groups is better. A significant observation is the larger proportion of poor-quality structures published in general-science journals.

E.N. Brown and S. Ramaswamy

L-Asparagine

***Acta Cryst.* (2007). E63, o3802-o3803 [doi:10.1107/S1600536807039505]**



A packing diagram of L-asparagine. Broken lines indicate the hydrogen bonds.

L-Asparagine is one of the fundamental natural amino acid residues in proteins. Amino acids very often have polymorphs. In this study, for the first time, a single-crystal structure determination of anhydrous L-asparagine is reported. The molecules are in their zwitterionic form. Although the carboxyl group is deprotonated, the distances of the two C—O bonds are significantly different due to different hydrogen-bond environments. The conformation of the side chain is *trans*, which distinguishes it significantly from that of the amino acid monohydrates.

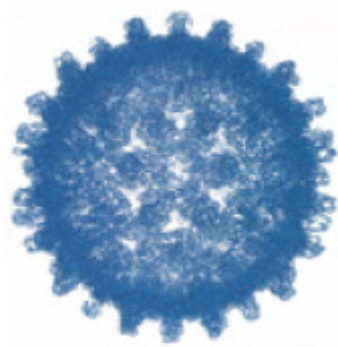
K. Yamada, D. Hashizume, T. Shimizu and S. Yokoyama

IUCR JOURNALS NEWS

Crystallization and X-ray analysis of the $T = 4$ particle of hepatitis B capsid protein with an N-terminal extension

Crystallization and X-ray analysis of the $T = 4$ particle of hepatitis B capsid protein with an N-terminal extension

Acta Cryst. (2007). F63, 642–647 [doi:10.1107/S1744309107033726]



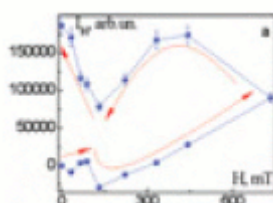
Electron density around the HBV capsid

The large hepatitis B virus (HBV) capsid has a molecular weight of about 4.25 MDa and comprises 240 copies of the core protein. Crystallization of a modified core protein containing an octapeptide N-terminal extension was found to be very dependent on temperature. The octapeptide extension was seen to protrude out from the surface of the capsid. This is consistent with the idea that N-terminal insertions can be exploited in the development of diagnostic reagents, multicomponent vaccines and gene delivery vehicles.

W.S. Tan, I.W. McNae, K.L. Ho and M.D. Walkinshaw

Polarized small-angle neutron scattering study of two-dimensional spatially ordered systems of nickel nanowires

J. Appl. Cryst. (2007). 40, s532-s536 [doi:10.1107/S0021889807005559]



Field dependence of the integrated intensity for perpendicular magnetic field

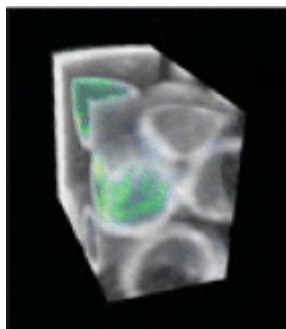
Magnetic and structural properties of two-dimensional spatially ordered systems of ferromagnetic nickel nanowires embedded into an Al_2O_3 matrix have been studied using polarized small-angle neutron scattering. An external magnetic field was applied perpendicular or parallel to the long dimension of the nanowires in order to reveal the anisotropic properties of the magnetic system. It is shown that, firstly, the magnetic-field-dependent scattering $I_H(q)$ provides new and principally different information as compared with the interference term $\Delta I(q)$. Secondly, two contributions to the interference term $\Delta I(q)$ (ascribed to the diffuse scattering and to the diffraction peaks) have different signs indicating different origins of the scattering objects. Thirdly, polarized SANS gives a detailed picture of the magnetization process, which could not be obtained by methods of standard magnetometry.

N.A. Grigoryeva, S.V. Grigoriev, H. Eckerlebe, A.A. Eliseev, A.V. Lukashin and K.S. Napolskii

IUCR JOURNALS NEWS

Three-dimensional chemical mapping by scanning transmission X-ray spectromicroscopy

J. Synchrotron Rad. (2007). **14**, 395-402 [doi:10.1107/S0909049507029962]

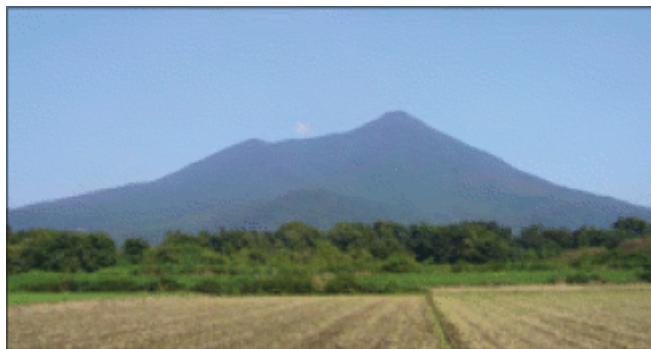


Three-dimensional representations of polyacrylate (green) and polystyrene (gray scale) distributions. Microsphere diameter is approximately 800 nm.

By using angle-scan tomography in a scanning transmission X-ray microscope three-dimensional (3D) chemical mapping was demonstrated. Information from near-edge X-ray absorption fine-structure spectroscopy at the oxygen edge was utilized to identify different chemical components in the sample. The technique is illustrated using mapping of a low density acrylate polyelectrolyte in and outside of polystyrene microspheres dispersed in water in a 4 μm diameter microcapillary. The 3D chemical visualization provides information about the microstructure that had not previously been observed in two dimensions.

G.A. Johansson, T. Tyliczszak, G.E. Mitchell, M.H. Keefe and A.P. Hitchcock

MEETING REPORT

AsCA'06/CrSJ**Epochal Tsukuba, Japan, November 2006**

Mount Tsukuba

The Joint Conference of the Asian Crystallographic Assn and the Crystallographic Society of Japan (AsCA'06/CrSJ) featured four Keynote lectures, eighteen microsymposia, and 331 poster presentations within a well balanced program covering all areas of crystallography.



M. Vijayan (President of AsCA)

Keynote lectures: S. Kitagawa (Japan): *Crystal and Functional Engineering for Unique Microporous Materials*; Zihe Rao (China): *Structural insights into SARS coronavirus proteins*. S. Iwata (UK): *Towards structure determination of human membrane proteins*; and C. Howard (Australia): *Structures and phase transitions in perovskites - sorting out the subtleties*.

Microsymposia covered the following topics: Structural genomics and high-throughput crystallography, Crystal engineering and supramolecular chemistry, Advances in powder diffraction, Macromolecular assemblies: protein/DNA/RNA, Inelastic X-ray scattering, Computational developments - SAD phasing, refinement, model building, validation, Materials science, Advancements in small angle X-ray scattering, Protein crystallization & post-crystal treatments - new tricks & tools, Magnetic structures, Electronic structure and bonding by X-ray diffraction, CBED, EELS, EXAFS, Membrane and membrane-associated proteins, Atomic resolution structure of biological macromolecules, X-ray and neutron scattering of strongly correlated electron systems, Cool structures, Nanotechnology: surface and interface, Disease related proteins, Dynamic aspects of molecular crystals.



Poster session

Three poster prizes sponsored by the IUCr, the RCSB PDB and CrSJ were awarded to young scientists: There was also a pre-meeting satellite on Theoretical Crystallography and Materials Science organized by The IUCr MaThCryst commission in cooperation with the IUCr Commission on Inorganic and Mineral Structures.



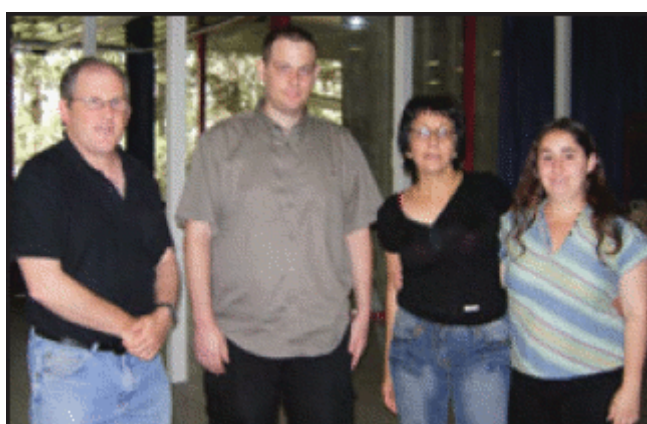
Participants of the AsCA'06 are trying to play Japanese drums (wadaiko) during the banquet. The next AsCA meeting will be held in Taipei in Taiwan R.O.C, November 4-7, 2007 (www.asca2007.tw).
Akiko Sekine

MEETING REPORT

ICA annual meeting

Haifa, Israel, May 2007

The Israeli Crystallographic Assn (ICA) held its annual meeting with more than 60 participants from six scientific institutions, on May 29th at the Technion - Israel Inst. of Technology in Haifa. The meeting began with a lecture by Frank Herbstein, the American Crystallographic Assn's 2007 Fankuchen Award Recipient. Other talks included macromolecular structural work on the binding of antibiotics to ribosome, p53 mutants, MitoNEET, a novel mitochondrial protein, phycocyanin at high resolution, the *M. tuberculosis* Cpn60.2 chaperonin, the carboxy-terminus domain of KCNQ1 and higher plant Photosystem I at 3.4 Å. Small molecules structural work was also represented with talks on TCNQ, porphyrins and co-crystals' synthons.



Left to right: N. Adir (chairman of ICA) with prize recipient C. Davidovich and his family.

The family of the late Ziva Berkovitch-Yellin has established an annual prize to be given at the annual ICA meeting, for excellence in crystallographic research by Israeli students. This year it was awarded to Chen Davidovich of the Weizmann Inst. of Science for his study entitled "Induced-fit tightens the binding of pleuromutilin antibiotics to ribosomes and remote interactions enable their selectivity" performed under the guidance of Ada Yonath.

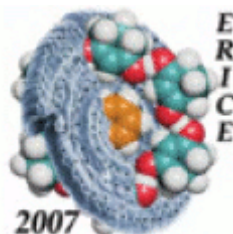
We gratefully acknowledge support of the meeting by Rigaku and Rhenium Inc., their representatives in Israel.

Michal Harel

MEETING REPORT

Engineering of crystalline materials properties: state-of-the-art in modelling, design, applications

Erice, Italy, June 2007



The basic idea behind this NATO Advanced Study Inst. (NATO-ASI) was to create an environment where researchers in different crystallographic specialities could exchange ideas about the design of new materials having tailor-made properties. New materials are already appearing in areas previously not considered accessible. In their introductory presentation to 118 participants from 35 countries, the three co-directors, Lia Addadi, Dario Braga and Juan Novoa stressed recent developments of this nature. Up to now, the rationale behind the design of new materials has been based on empirical observations. Sometimes these empirical rules fail and, as a result, progress in the production of new materials is hampered and depends upon serendipity as well as science. There is a growing consensus that a better understanding of structure-property relationships is needed. This is even more evident for materials simultaneously exhibiting several properties of technological interest. This NATO-ASI reviewed the current state-of-the-art for most materials of technological interest thus providing participants a complete review of materials design not only in his/her field of interest but of closely connected areas as well.

The scientific program was organized with one or more 1 hour talks on one type of material interspersed with talks on other types of materials. The 43 lectures were complemented by six short presentations. Two poster sessions, 32 posters each, were preceded by short summary presentations and followed by a three hour discussion period. A panel discussion was organized about open problems in materials design and future trends, including defense and security.



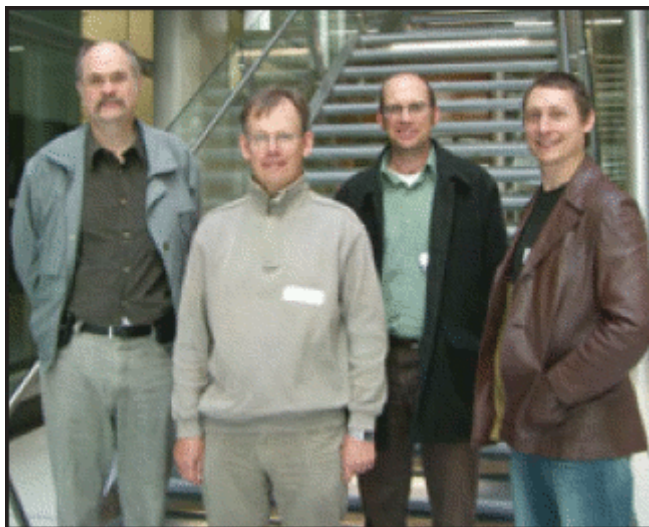
Participants at the 39th Course: Engineering of Crystalline Materials Properties in Erice, Italy
Each lecture was followed by ten minutes for questions. Student participation in all sessions was very high which resulted in the award of several prizes to young researchers during the closing ceremony; two awards went to students who asked the best questions during the discussion (Sathyanarayana Reddy Perumalla, (India) and Vincent Smith (South Africa)) and two went to the best poster presentations (Christina Capacci (USA) and Avital Levy-Lior (Israel)).

Paola Spadon

MEETING REPORT

1st Australian Workshop on solution scattering from biological macromolecules

Melbourne, Australia, July 2007



(From left) Keynote speakers: Dmitri Svergun (EMBL, Hamburg), Jan Skov Pedersen (Aarhus), Organizing Committee members: Terry Mulhern (Melbourne) and Haydyn Mertens (Melbourne).

The workshop, held at the U. of Melbourne, was organized by locals Terry Mulhern and Haydyn Mertens with financial support from the Australian Inst. of Nuclear Science and Engineering (AINSE), Bruker AXS, the Australian Synchrotron Project (Victorian State Government, Dept. of Innovation, Industry and Regional Development), the Australian Nuclear Science and Technology Organisation (ANSTO) and the U. of Melbourne.

The Workshop was proposed following discussions at an ASRP/Australian Synchrotron Users Meeting concerning the growing number of biological scientists in Australia using laboratory and synchrotron X-rays and neutron beams for small-angle scattering studies of biomolecular structure. These techniques are presently undergoing major development in Australia with new laboratory based SAXS instruments being installed, a new SAXS beam line at the Australian Synchrotron (completion mid 2008) and a new SANS instrument on the OPAL Research Reactor (completion late 2007).

Therefore, the aims of the workshop were to identify and bring together representatives of the embryonic Australian biological small-angle scattering community to facilitate collaboration, cooperation and the transfer of skills between research groups; and to provide specialist training to Australian biological scientists, particularly early career researchers skilled in complementary biophysical methods. Lectures and practical sessions were presented and guided by Jan Skov Pedersen (Denmark) and Dmitri Svergun (Germany). Twenty participants were selected from a long list of applicants from across Australia and New Zealand based at universities, research institutes and national research organizations. The workshop included lectures on the principles of small-angle scattering, data acquisition and analysis, and practical exercises on data analysis using programs from the ATSAS suite of software (www.embl-hamburg.de/ExternalInfo/Research/Sax/software.html/). Workshop tutors, Haydyn Mertens and Tracy Hanley (ANSTO) were kept busy with many questions from the enthusiastic participants. To facilitate discussion and promote on-going collaborations, the workshop concluded with a poster session and farewell drinks. During the poster session participants discussed their science with our invited speakers on topics that ranged from actin polymerisation, amyloidogenic aggregation of α -synuclein in Parkinson's disease, nuclear adaptor protein-protein interactions and the protein folding chaperone function of small heat shock proteins.



Attendees in the atrium of the Bio21 Institute, U. of Melbourne

The Organizing Committee would like to express their sincere appreciation to our invited speakers, Dmitri Svergun and Jan Skov Pedersen for the generous contribution of their time and course material. We would also like to thank our sponsors for their financial support and the Bio21 Inst. for hosting the workshop. The demand for places and the enthusiasm of the participants over the two days has encouraged us to plan to continue the workshop on a biennial basis.

Terry Mulhern and Haydyn Mertens

MEETING REPORT

Workshop on structure determination using powder X-ray diffraction

Lahore, Pakistan, August 2007



Crystallography is taught in Pakistan as a part of the solid state physics curriculum at the undergraduate and post-graduate levels. However, the treatment is superficial, teacher training is often inadequate, concepts such as symmetry, point and space groups are neglected and crystal structure determination is generally limited to the simplest structures. Furthermore, there are few diffraction facilities, computational resources are severely limited, and crystallographic software is generally unavailable. With this background in mind, the Khwarzimid Science Society (KSS) (www.khwarzimid.org) decided to organize a national workshop dealing with different aspects of crystal structure determination. The workshop on powder diffraction (XRD) was the first of its kind in the country. It was hosted at the Centre for Solid State Physics in Lahore where one of the organizers (S.A.Siddiqi) is a professor. The workshop was partially sponsored by Bana International and Bruker-AXS, Germany.



N. M. Butt in his inaugural address

The opening lecture “Diffraction Studies of Nanostructures” was given by N.M. Butt (Chairman of the Pakistan Science Foundation). As president of KSS and Chair of the Advisory and Organizing Committees, S.A. Siddiqi presented an overview of the KSS, which was established in 1997 and is arguably Pakistan’s most active society for the popularization of science.



Falak Sher describing the diffraction from body-centred iron

On the first day of the workshop the basics of crystallography were covered including symmetry, point and space groups, crystal lattices and the seven crystal systems. Special emphasis was placed on crystallographic notation problems students routinely face. Miller indices, planes, directions and fractional coordinates and the difference between lattices and structures were carefully described. An exercise worksheet was distributed. The second day dealt with diffraction and crystal structure determination. It featured marathon lectures by Falak Sher (Pakistan Inst. of Engineering and Allied Sciences) who methodically covered peak indexing, space group determination using systematic absences and the phase problem. M. S. Anwar (Lahore) covered the physical basis of diffraction focusing on the duality between real and reciprocal space, the Fourier and the convolution connections to crystal structure determination. On the final day, Falak Sher discussed the Rietveld method of refining trial crystal structures and demonstrated computer-based refinement methods, using the freely available program, GSAS with real examples. Menges Goetz (Bruker-AXS) described the instrumental, sample and background contributions to peak profiles and the “fundamental parameters” approach to analyzing peak profiles as it relates to refining crystal structures.



Menges Goetz, Nazma Ikram, Ijaz M. Ghauri, Saadat A. Siddiqi, Falak Sher and Jamil Khan.

The meeting was enhanced by lectures on related topics. Arshad Bhatti (Islamabad) lectured on “microscopic characterization of nanostructures” and Umair Manzoor from the same institute discussed “Electron microscopy and electron diffraction”. Speakers also made reference to neutron diffraction and synchrotron radiation throughout the lectures, adding to the value of the workshops.



Participants assessment forms indicated that the workshop was an overall success. Only 50 of more than a hundred individuals who applied could be accommodated. These were either users of XRD equipment, individuals who planned to buy new instruments under funding acquired from the Higher Education Commission (H.E.C.) of Pakistan or materials science students who were interested in learning about crystal structures. There were also a few H.E.C. Ph.D. scholars who were proceeding abroad to undertake research in the same subject. The attendees represented three (out of the four) provinces of the country and came from, for example: Sindh U (Jamshoro), Karachi U, U.E.T. Lahore, the Punjab U (School of Biological Sciences, Physics and Chemistry Dept, Centre of Excellence in Molecular Biology, Centre for Solid State Physics), Bahauddin Zakarriya U (Multan), PIEAS, Quaid-e-Azam U, Islamia U Bahawalpur, Government College of Technology (Bahawalpur), Dyal Singh College Lahore, PCSIR Labs Lahore, Pakistan Atomic Energy Commission, U of Peshawar, U of Agriculture (Faisalabad), NIBGE (Faisalabad), COMSATS(Islamabad), Vienna U (Austria).



Participants during one of the lectures

The participants were of varied backgrounds including physics, chemistry, biology, soil and environmental sciences, materials science, agriculture, engineering and geology. More details of the events, lecture notes and photographs can be accessed from the KSS website (www.khwarzimid.org). The KSS is planning an International Winter School on Crystallography in the year 2008 and formation of a Pakistan Union for Crystallography Research (PUCAR – literally meaning “a loud call for attention” in the Urdu language!) is envisioned in the very near future. This will definitely consolidate crystallographic research and teaching in the country and bring our standards in line with international practices.

M. Sabieh Anwar and S.A. Siddiqi

MEETING REPORT

Structural Methods in Chemistry, Biology and Medicine Workshop in memory of Yuri Struchkov

Chicago, USA, August 2007



Yuri Struchkov

The objective of the inaugural meeting of the Struchkov Prize Society was to focus on the fields of chemistry and chemical biology that utilize X-ray diffraction and molecular modeling to characterize novel materials and establish structure-property relationships in the worlds of small and large molecules. The meeting highlighted the scientific achievements and research of the colleagues who knew and collaborated with Prof. Struchkov and continue to use structural methods in their current work. The workshop enabled old friends and colleagues to forge new bonds and discover novel grounds for future interactions, idea exchange, and collaborations. The workshop was sponsored in part by the U. of Wisconsin-Madison and Bruker-AXS.

The program consisted of two full days of lectures, a reception dinner, and an excursion to the Bruker-AXS Madison, WI facilities on the third day. There were 12 speakers and 24 participants from Canada, Russia, Switzerland, and USA. It was a particularly memorable pleasure to see among the participants Yuri Struchkov's wife Irena Akhrem who traveled all the way from Moscow, Russia to attend and give an affectionate speech at the end of the meeting. The workshop combined saturated scientific and social programs with a very warm "family reunion" type atmosphere. The particulars of the conference are available at home.san.rr.com/struchkovprize/.



Left to right: Tatiana Timofeeva, Ilia Guzei, Alex Zolotoy, Sue Byram, Galina Belitskaya, Arkady Ellern, Inna Dubchak, Segrei Lindeman, Olga Lindeman, Tamara Kaftaeva, Mikhail Antipin, Irena Akhrem, Ewa

Skrzypczak-Jankun, Lev Zakharov, Galina Mednikova, Evgueni Mednikov, Chuck Campana, Jerzy Jankun, Alex Yanovsky, Victor Khrustalev.

The presentations covered a wide spectrum of topics ranging from the history of the society and evolution of the single crystal diffractometry software and hardware to photonic materials, palladium cluster chemistry, compounds for photodynamic therapy, to comparative and structural genomics and studies of human lipoxygenases. The highlight of the meeting was a comprehensive presentation by Prof. Michael Antipin on the development and history of the structural studies at the X-ray Structural Center in INEOS.

The first USSR diffractometer was purchased for the INEOS Xray Diffraction Group in 1971 and ever since the Roentgen rays emanating from INEOS have been influential in the scientific research. Since the mid-1970's the Structural Center has trained over 200 Ph.D. candidates and awarded over 20 Doctor of Science degrees to its members. The current structural investigations on several diffractometers are conducted by a team of 12-15 scientists who solve on average 1000 structures a year in addition to conducting charge density studies and theoretical computations.

After the untimely death of Prof. Struchkov in August 1995, a group of his former colleagues established the Struchkov Prize, an annual award for the young crystallographers from the Former Soviet Union countries. The first Struchkov Prize was awarded in the fall of 1997 and since then, 13 young scientists have received this honorable distinction, which includes a cash prize of about \$1,000. In addition to the main prize, which may be awarded to one or two individuals, a number of supplementary awards are given annually to a broader range of young FSU competition participants. In the first years of the Struchkov Prize, all awards were funded from a rather meager budget of the X-ray Structural Center in INEOS. In order to provide an independent source for the prize funding, in early 2000 the Struchkov Prize Society was established. The members of the international Struchkov Prize Society include former co-workers of Prof Struchkov now working in eight countries and other crystallographers who used to know Prof. Struchkov and collaborate with his lab. 100% of the members' annual contributions to the society subsidize the main prize and the supplementary awards. The latest information about the winners of the most recent Struchkov Prize 2006 can be found in IUCr Newsletter, 2007, Vol. 15, Issue 2, page 21. If you wish to support young crystallographers in Russia we invite you to become a member of the Struchkov Prize Society; please send your requests to StruchkovPrize@gmail.com.

During the closing remarks of the meeting Irena Akhrem reminded one of the maxims Yuri Struchkov used to repeat: "While the equipment you use is important, it is the people you work with, collaborate with, and compete against who take you to the next level." The success of the Struchkov Prize Society workshop in its own way confirms the great wisdom of this statement.

The next meeting is tentatively scheduled to take place in Santa Fe, USA, in August 2009.

Iliia A.Guzei, Alex I.Yanovsky

OBITUARY

Durward William John Cruickshank (1924-2007)



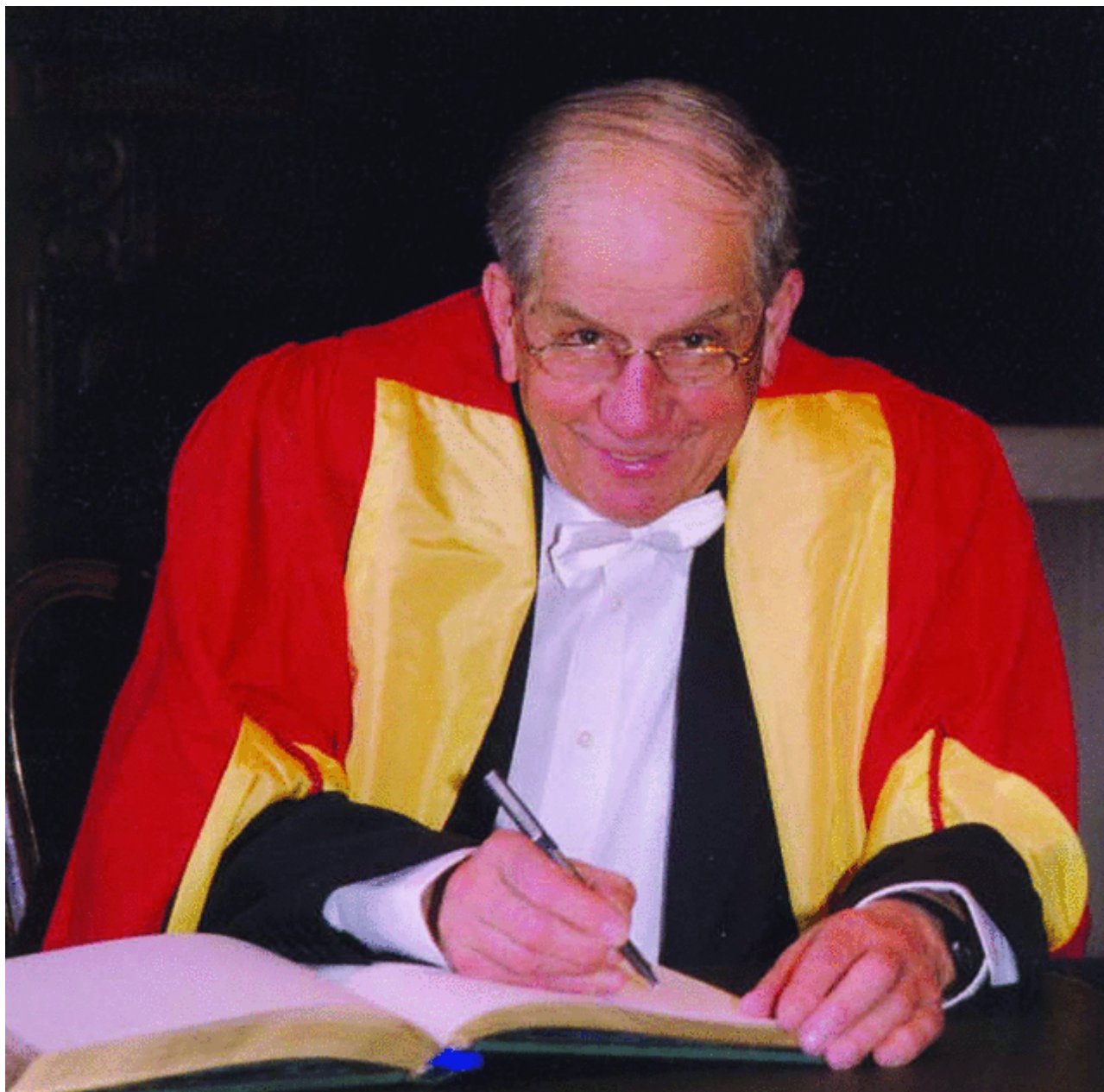
Crystallography in general and the IUCr in particular owe much to Prof. Durward Cruickshank FRS who died July 13, 2007 peacefully, of cancer, in his home village of Alderley Edge near Manchester. He 'retired' as Prof. of Theoretical Chemistry at the U. of Manchester Inst. of Science and Technology (UMIST) in 1983 but continued his research very actively until his death, with his last paper in *Acta Cryst.* (2007), **D63**, 906-922 still in press.

Durward Cruickshank transformed the precision of molecular structure determination in 3-dimensions by X-ray diffraction with research publications that span 60 years and that directly influenced at least some 450,000 chemical structures, the number currently held in the Cambridge Structure Database. Research on proteins occupied his attention throughout his last decade and the Cruickshank Diffraction Precision Index (DPI) indicator of the precision of a protein structure is now added regularly to many of the protein 3D structures deposited in the Protein Data Bank (PDB). His first paper in *Acta Cryst.* was published in Volume 1, pages 92-93. His final paper was on the determination of protonation states in proteins. He published over 80 papers in *Acta Cryst* from 1948 onwards on many topics in crystal structure refinement.

Cruickshank was an early pioneer in the use of digital computers, travelling from Leeds to Manchester, where Ferranti Ltd. commercialized the first stored-program digital computer, for round-the-clock crystallographic computation runs. He attended the 1950 Cambridge Summer School on Programme Design for Automatic Digital Computing Machines, one of the world's first summer schools on electronic computing, which introduced him to the principles of computer programming, machine order codes and binary arithmetic.

Durward was born in London on March 7, 1924 and educated at St. Lawrence College, Ramsgate. His career started at Loughborough College, now Loughborough U., as an engineering student, where he achieved an external degree from London U. in 1944, then worked until 1946 for the Admiralty on Naval Operations Research. He subsequently studied mathematics at Cambridge, "learning at the feet of Bondi, Hoyle, Boys and Dirac" as he would put it, and was awarded successively his BA (1949), MA (1954) and finally DSc (1961). His entry into the world of crystal structures began in 1946 when he joined E.G. Cox's (later Sir Gordon Cox) chemical crystallography group at Leeds U.

His first academic appointment was as Lecturer in Mathematical Chemistry at the U. of Leeds in September 1950. He became Joseph Black Prof. of Chemistry at Glasgow U. from 1962 to 1967, then was invited to UMIST in 1967 for appointment as Prof. of Theoretical Chemistry. Upon retirement in 1983, he became Emeritus Professor at UMIST and, latterly, at the U. of Manchester. He was appointed Deputy Principal of UMIST, 1971-1972, made a Companion of UMIST in 1992, and awarded an Honorary Degree by UMIST in 2004. He also received an Honorary DSc from Glasgow U. which named their Diffraction Laboratories after him.



His major contributions were formally recognized by the Royal Society which elected him a Fellow in 1979, also by other Prizes and Awards. Notably, he won the Chemical Society (now Royal Society of Chemistry) Award for Structural Chemistry in 1978 and the first Dorothy Hodgkin Prize of the British Crystallographic Assn (BCA) in 1991. He delivered the prestigious Bragg Lecture at Leeds U. during the annual BCA Conference of 1997, then to the public at the Royal Inst. in London where both Braggs, father and son, had worked. The Braggs are still the only father and son to be jointly awarded a Nobel Prize (in Physics, 1915, "for their services in the analysis of crystal structure by means of X-rays"). Cruickshank devoted much effort to the IUCr. He was elected IUCr Treasurer in 1966 at the General Assembly and Congress in Moscow for the period 1966 to 1969. The office of Treasurer was combined with that of IUCr General Secretary at the General Assembly and Congress in Stony Brook, NY, in 1969 where he was elected to serve in that joint office from 1969 to 1972. Under his guidance, the total financial assets of the IUCr grew steadily in this period to double their value, until his final year when the rising costs of publication and editing and a small erosion of the subscription base resulted in a small loss. These two offices together demanded and received an unusually high level of time and thought. His sage advice was subsequently sought by the IUCr on a variety of occasions. Cruickshank also served as an Editor of the 1992 IUCr Memorial Volume *P. P. Ewald and his Dynamical Theory of X-ray Diffraction* commemorating Paul Ewald, the founding father of the IUCr. Cruickshank's first contact with the

international crystallographic community was at the small Leeds symposium held in 1948 that attracted many participants from the X-ray Analysis Group conference held some days before in London which led to the formation of the IUCr. He is visible in the photograph in *Acta Cryst.* (1989). **A45**, 585.

Cruickshank also served the BCA as Vice President 1983–1985, was admitted an Honorary Member in 2003 and continued to contribute enthusiastically to BCA activities until his death. Durward Cruickshank was always upbeat, kind and helpful, courteous and gracious, inspiring the love and affection of family and colleagues, utterly trustworthy and sincere, and always available for advice. His deep insight into science extended to its history. He could also be quite firm. At the BCA's AGM in York in 2003, the question of introducing the category of 'Fellow of the BCA' arose. Durward spoke successfully against the motion, saying that such a hierarchical membership structure would put the egalitarian nature of crystallography in jeopardy if introduced.

Durward's wife Marjorie predeceased him. He is survived by a son and a daughter and five beloved grandchildren. He will be sadly missed by the whole community.

Sidney C. Abrahams and John R. Helliwell

MISCELLANY

The genesis of Fortran

The recent death of John W. Backus (1915-2007), who is considered to be the father of Fortran, elicited this account by David Sayre of the development of the computer language.



David Sayre

In 1954 Peter Friedlander and I were at the Johnson Foundation of the U. of Pennsylvania, working on the structures of benzantracene and 7,12-dimethylbenzantracene (7,12-DMBA), hoping to cast some light on 7,12-DMBA being a much stronger carcinogen than benzantracene itself. Peter, working on benzantracene, was finding a planar polycyclic structure, but 7,12-DMBA, which at that time was generally thought of by chemists as also being planar, was showing signs of crowding of the methyl groups and non-planarity. Wishing to check further, we decided to see whether least-squares 3D refinement would confirm this difference in the structures. At that time the only 3D least-squares program was Durward Cruickshank's program for the MADAM computer in Manchester England, but there was a closer machine, an IBM 701 at IBM's corporate headquarters in New York City, and IBM kindly offered a little time on the machine for the project. I wrote the program, and the non-planarity of 7,12-DMBA, as well as the planarity of benzantracene, was confirmed. (I discover now, in the modern literature on carcinogenicity, that the structure of 7,12-DMBA enables it to attach strongly to DNA, so that we had indeed in 1954 stumbled on at least some of the reason for its carcinogenicity.)

The reader might be interested to know how the programming was done in 1954. There was an assembly program for the 701, but sitting in Philadelphia I was unable to make much sense of it, and I ended by writing the program in absolute octal. In addition, the storage-tube memory of the 701 was not very reliable, so the practice was to have each major stretch of code in the program occur twice, and not proceed if the two answers did not agree. Warner Love was with me when we took the hand-punched deck of 0's and 1's to New York to try it, and it got stuck. That night one of us read the octal version aloud to the other, who was following on the cards. We found one mis-punched bit, and the next morning, when we corrected that, the program ran.



John W. Backus

I very much enjoyed the whole experience, so when I was asked if I would like to stay on with IBM I accepted, and early in 1955 found myself in a group which was writing software for the IBM 704, that was going to be the successor to the 701. Quite near to us was John Backus's group, working on Fortran for the 704. John, Harlan Herrick, Peter Sheridan, and Irving Ziller had worked out the main features of the Fortran language, and had taken it to the 701 users, who said that they liked it, but doubted if the Fortran processor would be able to produce really efficient programs from it. John and the others took this as a challenge, and started work. At some point in 1956 John asked to borrow me to help deal with a

situation which had developed. The opening Section 1 of Fortran (arithmetic statements; Harlan Herrick and Peter Sheridan) was nearing readiness, as were Section 2 (DO statements; Irving Ziller and Bob Nelson) and Section 3 (most remaining statements other than input/output; Dick Goldberg). Section 2, however, treated the DO statements as if the 704 came equipped with an unlimited number of index registers, whereas in reality it had only 3. John had borrowed Sheldon Best, a brilliant young programmer at MIT, to deal with that problem, and Sheldon had devised a brilliant Section 4 and Section 5 to do it. Lois Mitchell Haibt was programming Section 4, and Sheldon was partway through the programming of Section 5. At this point, however, his leave from MIT was ending. John therefore put together a new team (Dick Goldberg and myself) to finish Section 5, and we had it working by the spring of 1957. Roy Nutt, an outstanding programmer from United Aircraft in Hartford, then wrote Section 6 (input/output), and in 1957 the system was distributed, and was an immediate success. From the start it was noted for the efficiency of the programs which it created.

The Fortran group was the happiest work-group I have ever known. John Backus provided cheerful and highly intelligent leadership, and was always thoughtful of other people. Everyone engaged in the project loved it and believed in the importance of what they were doing. It has been a pleasure to re-live it now.

David Sayre

Taken from ACA RefleXions, Summer 2007