

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

Volume 12 · Issue 3

Collected archival edition

Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President



This issue of the Newsletter contains the call for papers for the XXth Congress and General Assembly of the IUCr. The Program Chair, Carlo Mealli, and the Program Committee, composed of representatives from all the Commissions of the Union, has prepared an exciting program that covers all areas of crystallography, from theory and instrumentation through applications in chemistry, biology, and material science and includes plenary lectures by internationally renowned scientists. Concern is often expressed that crystallography has become routine and is losing its luster. The growth of existing national crystallographic associations, the emergence of new ones, the success of the annual meetings of the IUCr regional affiliates, the increased volume of crystal structures in worldwide databases, the growth in publications based on crystallographic studies, and the fact that crystallographic schools and workshops are consistently overbooked all suggest that our science is alive and well and that rumors of its demise are premature. In the past year I have had the privilege of observing this growth and vitality in all parts of the globe.

The German Crystallographic Assn held its Annual Meeting in Jena, March 15-19, 2004. This highly successful meeting featured 400 abstracts, 600 attendees and over 20 exhibits. All areas of crystallography were represented in the three-day program that often had five concurrent sessions. The Max von Laue Prize was awarded to Wolfram Saenger, attendance at the business meeting was over 100, and two new working groups (on interfaces and on inorganics) were formed.

The newly formed Moroccan Crystallographic Assn (AMC) organized a school in El Jadida, May 10-15, 2004. There were 125 attendees, about one third of which were women and half were students. The school was conducted in French and the instructors were primarily from France (nine) with one from Denmark and four from Morocco. A short meeting report appears on page 14. The convention center and hotel in Marrakech will provide a superb site for the fourteenth meeting of the European Crystallographic Assn (ECA) to be held in Morocco in 2007. This will provide a wonderful opportunity to advance international cooperation and understanding. Crystallographers in Morocco and other emerging countries are concerned about the cost of the IUCr Journals and International Tables and some crystallographic databases and would like to be able to access them at reduced prices. The students are concerned about future support for science and where they will be able to pursue a career in crystallography. The IUCr has a Journals Grants program that addresses this problem and we need to find more ways to ease the entry of new nations into the benefits of the Union.

On the 30th Anniversary of the first Erice Meeting (on Direct Methods of Crystal Structure Determination) schools on Polymorphism, organized by J. Bernstein and R. Davis, and Electron Diffraction, organized by J. Labar, T. Weirich, and X. Zou, were held in Erice, June 7-24, 2004. On behalf of the IUCr, I had the honor of welcoming the 200 attendees from 33 countries at a joint opening session. The Erice Schools, which epitomize the spirit of the IUCr, have been brilliantly organized for 30 years by Ludovico Riva di Sanseverino (and recently with Paola Spadon). They bring people from all nations together to educate the next generation of crystallographers.

The Asian Crystallographic Assn (AsCA) Meeting was held June 27-30, 2004 in Hong Kong. The 280 attendees came from 20 countries. There was a full three-day scientific program with eight plenary lectures and 70 oral presentations in three parallel sessions and 209 poster presentations. There was

good representation in the program from powder, materials, and macromolecular science. Four of the 15 exhibitors, sponsored major functions [opening reception (PANalytical), a boat trip with dinner (Bruker Nonius), a banquet (Rigaku), and a closing champagne luncheon (MAR Research). (After the first thirteen courses at the Rigaku banquet, I went on a hunger strike). Crystallographers in Bangladesh, Singapore, and The Philippines who attended the meeting expressed interest in joining the IUCr. AsCA currently has 18 countries as members, only eight of which are IUCr member countries. In the past AsCA has met every three years and held a council meeting at the IUCr Congress. In 2003, a joint meeting of AsCA and the Society of Crystallographers in Australia and New Zealand (SCANZ) initiated a new policy of meeting every third year in conjunction with a national meeting of a member country. The next of these joint meetings will be in 2006 when AsCA will meet jointly with the Crystallographic Society of Japan (CrSJ) in Tsukuba. Problems with no shows, keeping student fees low, strengthening ties between the regional affiliates, improving the AsCA website, and finding ways to sustain continuity were discussed at the business meeting.

The America Crystallographic Assn (ACA) meeting in Chicago, IL, July 17-22, 2004 was the second largest in ACA history (1213 participants). Among the highlights of the program were a crystal growth symposium honoring Fankuchen Award winner, A. McPherson; the first Supper Award given to N.-H. Xuong, recognizing his exceptional contribution to crystallographic instrumentation; the Margaret Etter Early Career Award presented to L. MacGillivray; and the Trueblood Award presented to R. Marsh. The Transactions symposium "Crystals in Supramolecular Chemistry" and the symposia honoring MacGillivray and Marsh were ample proof that chemical crystallography remains a robust and growing area. Full reports on these and all sessions of the ACA meeting appear in the ACA Newsletter and on its website. The program also included a full day workshop designed for high school students and teachers. The program was co-sponsored by the ACA and the RCSB PDB with H. Berman, Director of the RCSB, providing ideas and guidance.

Highlights of the ECA meeting held in Budapest, August 26- 31, 2004, included the awarding of the first Max Perutz Prize to G. Sheldrick for his contribution to automated methods of phase and structure determination and a session in memory of Jacek Gróchowski, whose tragic death is a blow to Polish crystallographers and his many friends throughout the world. There were five concurrent sessions throughout the four-day meeting. The 60 attendees at the ECA council meeting included representatives from all current and potential member countries and the 13 special interest groups that organize the program for the annual meetings. ECA Chairman, H. Fuess described the renaming of the ECA Prize to the Perutz Prize, the planned periodic review of the structure and activities of the individual SIGs and possible reorganization of the program committees for future ECA meetings.

In light of the remarkable level of activity in the field of crystallography reflected in these national and international meetings, and the superb program for the XXth Congress and General Assembly outlined in the pages of this Newsletter, I urge all 15,000 readers of this Newsletter to make plans to be in Florence in August 2005.

Bill Duax
 duax@hwi.buffalo.edu

EDITORIAL

Scientific publishing in the 21st Century



Scientific publishing is undergoing a revolution. I only have to look at my own department to see the effects. Last year, after existing as long as the department itself, our local branch of the university library was closed. Besides providing a salary savings and releasing precious floor space for other purposes, the closure resulted principally from a change in the reading habits of its patrons. Access to the World Wide Web brings research papers to every individual's desktop provided they are fortunate enough to have access to a high speed internet connection. As a result fewer and fewer people are reading journals from cover-to-cover each week other than the popular magazines, such as *Nature* and *Science*. Most researchers rely on alerting services to bring relevant articles to their attention which they then access over the internet. The result of this behavior is that many publishers are facing a slow but steady decline in the number of subscribers. There are fewer libraries competing for what seems to be an ever increasing number of publications. All this directly affects the International Union of Crystallography which relies for much of its financial support on the health of its publishing enterprise.

Furthermore, while the community at large and granting agencies in particular (at least in my country) are placing increasing emphasis on the impact factors of journals, one can reasonably argue that changing reading habits have rendered the impact factors of journals less relevant. If people only select articles chosen from various abstracting and citation services according to key words and phrases and access the copies electronically then the 'impact' of the journal as a whole should have little relevance. For individual authors seeking recognition it should be the number of citations their papers receive that is important not the number a particular journal receives on average. I hope this is some little comfort to the hard working editorial staff of *Acta Crystallographica* who continue to seek ways to improve the already quite good impact factors of the *Acta* family of journals. Review articles and papers describing widely used experimental procedures characteristically receive the highest numbers of citations, but are these the most 'important' contributions to the scientific literature?

Moves to enforce a regime whereby work funded by government and charitable organizations is made freely available has profound implications for the financial viability of scientific publishing. The consequences are not restricted to commercial publishers who need to profit from their enterprises but also publications of learned societies who still require that their publishing ventures at least break even financially and in some cases profit to fund other aspects of the society's work. The National Institutes of Health, U.S.A. (NIH) is taking a leading role in encouraging open publication by proposing to mandate free availability of all work funded by the NIH after six months from publication. The NIH is currently seeking comments on its proposals (<http://grants.nih.gov/grants/guide/notice-files/NOT-OD-04-064.html>). A recent report by a select committee of the House of Commons in Britain (www.publications.parliament.uk/pa/cm/cmsctech.htm report of 20th July 2004) recommends that individual institutions maintain repositories for all experimental data and that they make these freely available. Many of these

suggestions appear to undervalue the role of peer review in the publishing process. *Acta Crystallographica* has put forward suggestions on open access (<http://journals.iucr.org/iucr-top/iucr/stcttee04.html>) and is willing to work with the NIH and others to achieve their aims in a sustainable way. Other means to make works freely accessible by requesting payments from authors of individual papers to provide open access are already available from some publications including *Acta Crystallographica*. The government in Britain has funded a trial with *Acta Crystallographica* whereby they have made a single payment to the journal to provide open access for all publications by British academic researchers. This mode of funding open access has the advantage that the journal can still receive sufficient funding to cover the considerable editorial costs involved in publishing a high quality publication such as *Acta Crystallographica*.

As the world of publishing faces the challenges outlined above, the field of macromolecular crystallography is giving publishers a number of new challenges of its own. High throughput methods and the funding of initiatives in structural genomics, stand to rapidly increase the number of solved protein structures. Furthermore, given that these proteins may have no well defined biological role, publication in traditional journals may not be possible. However, the structures will still be deposited in the Protein Data Bank (PDB). Is there any value in further publication? The taskforce on publication, convened by the NIH and the Wellcome Trust, concluded that there was indeed additional value in a refereed publication even if most of the result was encapsulated in the data bank deposition. The added value would come in the form of commentary by the authors placing their structure in the context of existing knowledge and by the process of peer review which would ensure standards of the published work. The PDB itself does not seek to impose any standards on deposited data. Tools are provided for structure evaluation but structures which fail to meet preset standards are not excluded from deposition.

Acta Crystallographica is revising its family of publications to meet the challenges outlined above. *Acta Crystallographica* Section F will be an all electronic counterpart to *Acta Crystallographica* Section D for the publication of communications in macromolecular crystallography in much the same way as Section E complements Section C. Section F will publish structure communications, crystallization notes, and the results of structural genomics studies. The all-electronic format will provide wide scope for the use of color illustrations and movies. Papers will be refereed and application has been made to PubMed and ISI for abstracting and for the accumulation of citation data. A new and exciting feature planned for Section F is the easy transfer of data from the PDB submission (enhanced to capture all the experimental details) via the author to the journal in a form that is easily organized into tables ready for publication. Implementation of the new data types has involved a close collaboration with the staff of the Research Collaboratory for Structural Bioinformatics (RCSB PDB). This new procedure will aid authors by highlighting required information absent from the submission and speed up the refereeing process. Referees will also have access to the structure validation data. Section D will continue to publish fully described macromolecular structures and papers on new methods including those relating to crystallization. *Acta F* will publish the short crystallization notes formerly in Section D.

The first issue of *Acta Crystallographica* Section F will be published in January 2005 and you are invited to submit papers now. Papers are made available as soon as they are accepted and the first of these may be viewed now (<http://journals.iucr.org/>).

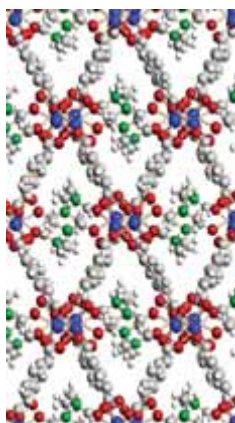
Mitchell Guss, University of Sydney, Australia

IUCR JOURNALS NEWS

Synchrotron charge-density studies in materials chemistry: 16 K X-ray charge density of a new magnetic metal-organic framework material, $[\text{Mn}_2(\text{C}_8\text{H}_4\text{O}_4)_2(\text{C}_3\text{H}_7\text{NO})_2]$

Synchrotron charge-density studies in materials chemistry: 16 K X-ray charge density of a new magnetic metal-organic framework material, $[\text{Mn}_2(\text{C}_8\text{H}_4\text{O}_4)_2(\text{C}_3\text{H}_7\text{NO})_2]$

Acta Cryst. (2004). A60, 382–389 [doi:10.1107/S010876730401699X]



The crystal structure of $\text{Mn}_2(\text{C}_8\text{H}_4\text{O}_4)_2(\text{C}_3\text{H}_7\text{NO})_2$ at 16(1) K viewed along the *a* axis. The DMF molecules bonded directly to manganese occupy the voids.

Metal organic frameworks, MOFs, are of high current interest due to their gas storage abilities. This paper focuses on the physical properties of a magnetic Mn-based MOF, and it presents the 16(1) K structure and charge density, the heat capacity and the magnetic susceptibility of

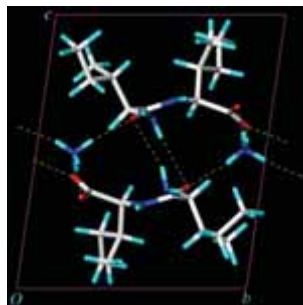
$\text{Mn}_2(\text{C}_8\text{H}_4\text{O}_4)_2(\text{C}_3\text{H}_7\text{NO})_2$. Formal charge counting based on the crystal structure predicts two manganese atoms with +1.75 *e* charge and one with +2.50 *e*, while the topological analysis of the charge density results in Bader charges of +2, as predicted from synthesis. The effective magnetic moment is observed to be 5.96 μ_{B} , which is in excellent agreement with the experimentally determined charge density having close to one electron in each *d* orbital.

R. D. Poulsen, A. Bentien, T. Graber and B. B. Iversen

IUCR JOURNALS NEWS

A crystallographic titration of the dipeptide L-isoleucyl-L-isoleucine

***Acta Cryst.* (2004). B60, 569–577 [doi:10.1107/S0108768104014569]**



Structure of L-isoleucyl-L-isoleucine as an anion in the ammonium salt, the first of this kind for an amino acid or a peptide. Crystals were prepared by slow evaporation from a $\text{NH}_3(\text{I})$ solution.

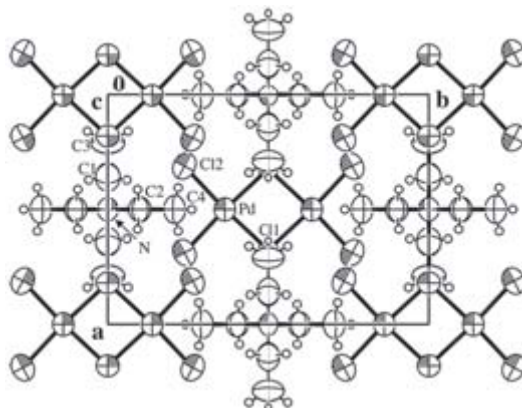
The dipeptide L-isoleucyl-L-isoleucine has been crystallized in four different protonation states including as a cation, a zwitterion and an anion as well as a dimeric cation where two peptide molecules, linked by a strong $\text{COO}\cdots\text{H}\cdots\text{OOC}$ hydrogen bond, share an overall positive charge of +1. The paper on this unprecedented series of crystal structures highlights differences in hydrogen bonding capabilities, conformational properties and molecular packing arrangement. The packing is particularly interesting for the cationic form (as a nitrate), which forms a nanotubular structure. Channels running parallel to a trigonal axis have a 4.0 Å van der Waals' diameter.

C. H. Görbitz

Two phases of bis(tetraethylammonium) di- μ -chloro-bis[dichloropalladium(II)]

Two phases of bis(tetraethylammonium) di- μ -chloro-bis[dichloropalladium(II)]

Acta Cryst. (2004). C60, m426-m430 [doi:10.1107/S0108270104016725]



A view of the unit cell at 292 K along the *c* axis. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

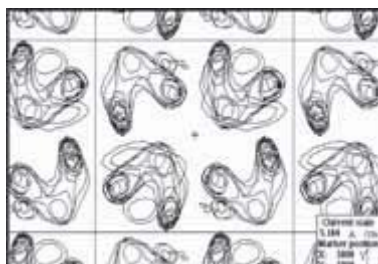
The article describes two phases and a phase transition at ~153 K in the title compound $[\text{N}(\text{C}_2\text{H}_5)_4]_2[\text{Pd}_2\text{Cl}_6]$. This compound is chemically related to $(\text{NH}_4)_2[\text{PdCl}_4]$ and to $[\text{N}(\text{CH}_3)_4]_2[\text{PdCl}_4]$ where phase transitions depending on temperature also occur and the structures of which were previously determined. The low-temperature phase of the title compound is twinned as a consequence of the phase transition ($Immm \rightarrow I2/m$). The most interesting structural feature is the presence of C-H...Cl interactions as short as ~2.80 Å. Vibrational spectroscopy confirmed that there are C-H...Cl hydrogen bonds in the structure.

J. Fábry, M. Dusek, K. Fejfarová, R. Krupková, P. Vanek and I. Nemec

IUCR JOURNALS NEWS

Ab initio phasing based on topological restraints: automated determination of the space group and the number of molecules in the unit cell

***Acta Cryst.* (2004). D60, 1519-1526 [doi:10.1107/S0907444904014969]**



An attempt of phasing in an incorrect space group results in a nonsense image of the structure (right); compare with the image obtained for the correct choice of the space group (left).

Direct phasing starting from low resolution is complementary to conventional phasing methods and may be efficient when these techniques fail or are inapplicable. The approach described here uses a single set of structure factor magnitudes and the expected number of 'blobs' visualized in the corresponding Fourier maps (each of the 'blobs' stands for a molecule or a molecular domain). The method discriminates between the correct and incorrect assignment of this number, therefore providing a way to determine the number of molecules in the unit cell as well as to select the correct space group in ambiguous cases.

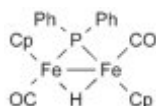
L. Urzhumtseva, N. Lunina, A. Fokine, J.-P. Samama, V. Y. Lunin and A. Urzhumtsev

IUCR JOURNALS NEWS

μ -Diphenylphosphido- μ -hydrido-bis[carbonyl(η^5 -cyclopentadienyl)iron(II)]

μ -Diphenylphosphido- μ -hydrido-bis[carbonyl(η^5 -cyclopentadienyl)iron(II)]

***Acta Cryst.* (2004). E60, m1284-m1285 [doi:10.1107/S1600536804019919]**

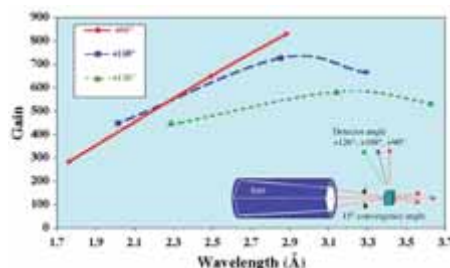


The desire to understand the mechanism for the seemingly trivial reduction of H^+ to H_2 by hydrogenase enzymes has resulted in extensive research activity in the field of metal-hydride chemistry. Applications of such electrocatalytic processes are particularly important in view of current efforts towards a Hydrogen Economy, where iron hydride complexes may serve as cost effective alternatives to platinum catalysts in fuel cells. The title compound is a rare example of a crystallographically characterized di-iron monohydride and displays high symmetry within the planar heterocycle. The cyclopentadienyl/carbonyl groups are in a trans geometry, which is unusual for this class of compounds.

A. Decken, C. D. Craig and F. Bottomley

Convergent-beam neutron crystallography

J. Appl. Cryst. (2004). **37**, 778–785 [doi:10.1107/S0021889804015882]



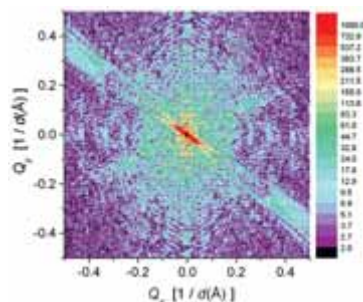
Intensity gains with the optic for the three lowest-order nickel powder diffraction peaks in detector banks at three different scattering angles as a function of neutron wavelength.

Focusing polycapillary optics enhance diffraction intensities for neutron convergent beam time-of-flight crystallography with a broad wavelength bandwidth. An optic with focal distance of 15 mm and beam convergence of $\sim 15^\circ$ has a focal spot width of 100 μm for 3.2 Å neutrons. For an MnF_2 single-crystal sample as small as 0.01 mm^3 , we observe an expected intensity gain of ~ 100 for a 020 Bragg peak. Measurements on a powder diffractometer show diffracted beam intensities for Ni powder with expected gains in excess of 500 for samples of this diameter. Backscattering geometry minimizes degradation of resolution for this large beam convergence.

W. M. Gibson, A. J. Schultz, J. W. Richardson, J. M. Carpenter, D. F. R. Mildner, H. H. Chen-Mayer, M. E. Miller, E. R. Maxey and R. Youngman

Diffractive imaging of nonperiodic structures using coherent X-rays

J. Synchrotron Rad. (2004). **11**, 432–438 [doi:10.1107/S0909049504016772]



Simulated coherent X-ray diffraction pattern of a nonperiodic object consisting of 2894 gold atoms in a 10 nm cube, using a proposed synchrotron source at Cornell. Statistical noise is included in the signal. This oversampled diffraction pattern has been successfully phased to retrieve the original object using an iterative algorithm.

Coherent diffractive X-ray imaging is a microscopic technique for imaging noncrystalline objects at high spatial resolution. In this article, the authors present a simple method to estimate the coherently scattered signal for a specimen of a constant volume. A simulated case study (figure) confirms the estimated flux requirement. Combined with empirical radiation damage data in the literature, it is concluded that the resolution could reach ~ 5 nm for biological specimens of 100 nm in size, and close to atomic resolution for material science applications in diffractive imaging experiments. Larger specimens or an array of same objects would enhance the scattering signal and thus increase the achievable spatial resolution.

Qun Shen, Ivan Bazarov and Pierre Thibault

MEETING REPORT

Errors and pitfalls in single crystal structure analysis

Kiel, Germany, July 2003



Participants at the First Kiel Workshop on 'Errors and Pitfalls in Single Crystal Structure Analysis'. The First Kiel Workshop on 'Errors and Pitfalls in Single Crystal Structure Analysis' was held July 14-16 in Kiel, Germany.

X-ray diffraction on single crystals is one of the most common and precise methods of structure determination. The relatively small experimental expenditure for a routine X-ray structure analysis as well as the revolution in data processing has led to an enormous spread of this method in recent years. However, sometimes problems occur that impede data collection or structure solution or yield an unusual structural model. Even if a structure seems to be successfully determined, errors might have occurred which are difficult to detect. All these problems were addressed at the First Kiel Workshop which took place from 14-16 July 2003 at the University of Kiel in Northern Germany. Only participants were admitted who had already gained some practical experience with structure determination. The workshop was organized by Christian Näther from the Institute of Inorganic Chemistry (Kiel) together with Michael Bolte and Ernst Egert from the Institute of Organic Chemistry and Chemical Biology at the Goethe-University (Frankfurt am Main) as a common activity of the German Crystallographic Association (DGK) and the German Chemical Society (GDCh).

The workshop was divided into five topics: problems with the determination of the crystal system, the Laue symmetry and the space group; problems with structure solution; problems during structure refinement; twinning; precision, accuracy and assessment of the quality of a structure determination. Each topic was dealt with during half a day starting with introductory lectures. Then the participants had to tackle structural problems using standard software as described in detail in the workshop manual. Finally the solutions were discussed with the whole group.

Assessment by the participants afterwards was unequivocally positive and we still receive e-mails with nice comments. For example, a two-year old structure was recently solved with the knowledge acquired in the course.

Further information is available at www.chemkrist.de (unfortunately only in German like the course itself).

Christian Näther, Michael Bolte and Ernst Egert

MEETING REPORT

50 years of collagen triple helix: a celebration of science

A tribute to G. N. Ramachandran



Abdul Kalam, President of India, at the podium. Sitting, left to right are T. Ramasami, S.P. Thyagarajan, R.N. Mashelkar, Kapil Sibal, V.S. Ramamurthy, and S.K. Brahmachari.

G. N. Ramachandran (GNR) was an outstanding crystallographer and structural biologist. The model of collagen he developed has stood the test of time and has contributed greatly to understanding the role of this important fibrous protein. His pioneering contributions in crystallography, particularly in relation to methods of structure analysis using Fourier techniques and anomalous dispersion, are well recognized. The Ramachandran plot remains the simplest and most commonly used descriptor and tool for the validation of protein structures. He received many prizes, including the 1999 Ewald Prize of the IUCr.

His first major contribution to structural biology was the proposal, made along with Gopinath Kartha, of the triple helical structure of the fibrous protein collagen. The proposal was published in *Nature* in 1954. A symposium entitled '50 years of triple helix: a celebration of science' was organized by S.K. Brahmachari, M. Bansal, and T. Ramasami in New Delhi on August 7, 2004, to commemorate the 50th anniversary of this event. The symposium and the production of a documentary on the life and work of GNR, were supported by the Council of Scientific and Industrial Research (CSIR) and the Dept. of Science & Technology (DST). R.A. Mashelkar, Director General of CSIR, gave the keynote address. Taking examples from his own research on polymers, he emphasized the importance of being alert to deal with unanticipated and unusual results. V.S. Ramamurthy, Secretary, DST, presided over the inaugural function.

Three of the speakers were former students of Ramachandran. M. Bansal, his last graduate student, worked on the role of hydroxyproline in collagen and traced the history of the discovery of the coiled coil triple helical structure of collagen. The way Ramachandran and Kartha, working in virtual isolation at the U. of Madras, conceptualized the collagen model using scanty biochemical and X-ray data, was truly remarkable. Her own work led to the appreciation of water-mediated hydrogen bonds involving hydroxyproline.

C. Ramakrishnan, a co-architect of the Ramachandran plot, then described how the controversy regarding the so-called short inter-atomic distances in the collagen model structure, led to a thorough examination by the GNR group of the minimum permitted distances between different non-bonded atoms. From crystal structure data, they were found to be considerably less than the sums of the appropriate van der Waals radii. This re-examination led to the Ramachandran plot which graphically illustrates the restrictions on polypeptide conformation. This was at a time when the structure of only

one globular protein had been determined. Now, after forty years and thousands of structure determinations, the Ramachandran plot remains a very important tool for describing and validating protein structures.

A.S. Kolaskar, another student, discussed the contribution of Ramachandran to the development of computational biology and bioinformatics. His own work with GNR was concerned with the non-planarity of the peptide unit consequent to the pyramidal nature of the amide nitrogen. The non-planarity was established through quantum chemical calculations and analysis of crystal structure data.

M. Vijayan, former head of the Molecular Biophysics Unit (MBU) established by GNR at the Indian Inst. of Science, Bangalore, dealt with the GNR legacy in crystallography. He referred to GNR's contribution to the use of anomalous dispersion for structure analysis. Much of Ramachandran's contributions were theoretical or computational in nature. He was keen on initiating biological macromolecular crystallography in India, but it could not be done during his active professional life. However, he lived to see the MBU, one of the two schools he established, play a leadership role in the development of macromolecular crystallography in India.

The Central Leather Research Inst. (CLRI), Chennai (formerly Madras), is situated next to the laboratory in which GNR worked during the 1950s and the 1960s. The original sample of collagen used by GNR in his X-ray diffraction experiments was in fact supplied by CLRI. The current Director of CLRI, T. Ramasami, described this association as well as currently available collagenbased materials, particularly those developed at his own Institute. A large number of diseases associated with collagen malfunctioning have been identified. The presentation of D. Balasubramanian was concerned with these diseases while S.S. Sriramachari spoke on diseases related to the effect of dietary protein on collagen.

The last scientific session was related to genomics. H. Yang (Beijing Genomics Inst.) gave an overview of the activity in this area in China. He described how their progress from sequencing one percent of the human genome to 100 percent of the rice genome. The last talk was by S.K. Brhamachari, the main organizer of the meeting. He recalled his early experimental work pertaining to the hydroxylation of proline, as a graduate student of the MBU. He went on to discuss the major computational genomics and bioinformatics efforts, which are being pursued in conjunction with experimental studies, at his institution in Delhi.

A highlight of the symposium was the participation of the President of India, Abdul Kalam. Kalam made major contributions to Indian space and defense efforts before becoming the president. Kapil Sibal, the new Minister for Science and Technology, discussed the Indian government's commitment to scientific research and promised to remove the bureaucratic bottle necks that can get in the way of its meaningful pursuit. The President also interacted in a question-answer session with students.

Ramachandran's active research career in structural biology ended almost 25 years ago, well before his death in 2001, yet he remains a vibrant presence in the field. He was arguably the most outstanding scientist to have worked in independent India. He demonstrated how international science could be decisively influenced even when working under difficult conditions in less well-endowed neighbourhoods. The August 7 symposium was indeed a fitting tribute to his memory.

M. Vijayan

MEETING REPORT

Turkish Crystallographic Association

Samsun, Turkey, April, 2004



Participants of the first National Meeting of the Turkish Crystallographic Assn held in Samsun, Turkey, April 22-24

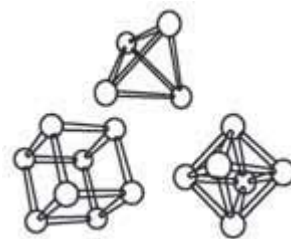
The first National Meeting of the Turkish Crystallographic Association was held in Samsun, Turkey, April 22-24, 2004 at Ondokuz Mayıs U. which received a new Stoe Imaging Plate Diffractometer System, STOE IPDS II, last year. 102 crystallographers from 12 different universities participated at the meeting. This meeting featured 8 invited lectures, 14 oral and 41 poster presentations. The topics of the invited papers were: Single Crystal Diffractometers and Detectors (J. Richter), The Story of STOE IPDS II Diffractometer at the Ondokuz Mayıs U. (O. Büyükgüngör), SESAME - Synchrotron Light for Experimental Science and Applications in the Middle East (D. Ülkü), Universal Behaviour of Magnetic Phase Transitions of $R_1-xR'_xMn_2X_2$ (R: rare earth element, X: Si or Ge) Compounds in the Mn sublattice (Y. Elerman), Powder Structure Solution (E. Kendi), The Agreement Between Ligand Binding Types Obtained with IR and X-ray Single Crystal Results (V. T.Yılmaz), Macromolecular Crystallography by Synchrotron Radiation: Structure of Daffodil and Lentil Lektin Complexes (S. Özbey), New Approaches in Science Teaching (Hüseyin Soylu). The best poster presentation an award was given to Gökhan Kastas at the closing ceremony.

Social activities included a visit of the Atatürk Museum and Bandırma boat which is a symbol in Turkish history for the beginning of the independence war in 1919. This really successful meeting ended with a farewell dinner with a splendid view of Kızılırmak River. The 2005 meeting of Turkish Crystallographic Association will be held at Kayseri, Erciyes U.

Engin Kendi

MEETING REPORT

Slovenian-Croatian Meeting

Bovec, Slovenia, June, 2004

The 13th Slovenian-Croatian Crystallographic Meeting followed the tradition of the previous ones to be yet another example of joining people together in science and pleasure. Sixty seven crystallographers with accompanying persons predominantly from Croatia and Slovenia, have proved once again that we are able to maintain a reasonably high scientific level of crystallographic research and at the same time maintain friendships inside our crystallographic community.



The lectures were followed with great interest

There were four plenary lectures: R. Loris (Brussel, Belgium) Structural Basis of Plasmid Addiction and Programmed Cell Death in Bacteria; D. Turk (Ljubljana, Slovenia) Roles of Papain-Like Cathepsins in Immune System Response: Exclusive Interactions as the Other Face of Selectivity; J. Sieler (Leipzig, Germany) Architecture and Design of New Porous Networks; A. Mogus-Milankovic (Zagreb, Croatia) Structure and Properties of Phosphate Glasses, and over forty oral presentations.

There were 61 participants from nine countries. Plenary lectures included modern topics from crystal engineering and protein structures to the practical use of modern and new materials. Short presentations included the crystallographic subjects of proteins, organic and organometallic structures, inorganic structures, coordination compounds, metallic alloys and oxides, minerals, powder diffraction, microporous material, zeolites, etc.

Our thanks to our permanent Honorary Chairmen, L. Golic (Ljubljana) and B. Kamenar (Zagreb), who started our meetings in 1992 after the disintegration of Yugoslavia and have continued to organize these annual meetings. We wish them all well and good health in the future.



There was an afternoon trip to Kobarid World War I Museum and the fortress Kluze. The afternoon excursion was to the museum of World War I in Kobarid and to the fortress Kluze in the valley of the Soca river. The beautiful Trenta Valley, from the emerald river to the summit of the mountains was the scene of the cruel wars of 1916, when in these parts the Austrian and Italian armies faced each other, bleeding from violent attacks and counterattacks, while down in the valley the young Hemingway was witnessing scenes of horror and turning his bitter experience into an inspiration for his famous novel *A Farewell to Arms*. Those mountains towering above the Soca river (Isonzo in Italian) were destined to see twelve bloody battles, some of which are counted among the hardest battles of the First World War. These mountains lining the Soca Valley long ago became a wall between the two worlds, but now the border has disappeared, since Slovenia joined EU in May 2004.

It is a fact that crystallographers from Slovenia and Croatia, with participants from other countries, have been gathering now for 13 years, since 1992. There is an increasing impact of crystallography on science in our developing countries, as well as in the world.

With great pleasure we greet our guests each year from abroad and we try as much as possible to keep the meeting without a registration fee, which is unique in the world of conferences. Next year's meeting will be organized in June 2005 at the Istrian coast in Croatia. There is an open invitation to all bona fide scientists and friends to attend the 14th Croatian-Slovenian Crystallographic Meeting. For further information, contact S. Popovic (Zagreb, Croatia) at spopovic@phy.hr.

S. Popovic

Closing remarks by S. Popovic (Zagreb, Croatia)

Now it is my turn to say several words at the closing point of our meeting, on behalf of the honorary chairmen, Professors Goliè and Kamenar, on behalf of the co-chairmen and my friend V. Leban, and on behalf of SCS and CCA. We now say good bye and good luck to each other. This meeting has taken part in a beautiful place, created by Nature, and I hope all of us have enjoyed our stay here.



Plenary lecturers (left to right): J. Sieler, R. Loris, A. Mogus Milankovic, and D. Turk.

This meeting, I hope you share my opinion, has been a very successful meeting, as were the previous ones, scientifically and socially, offering a friendly and domestic atmosphere. We listened to four very nice plenary lectures, concerning modern approaches in crystallography. Forty-four short oral contributions were presented with different but contemporary topics in crystallography, including both data acquisition and interpretation. I would like to express our gratitude to the general lecturers, and to all of you who have come here to attend this meeting. There have been 61 active participants and 7 accompanying persons from 9 countries.

I would also like to express our thankfulness to the sponsors, who helped this meeting, because without their support the meeting would not have been possible. The Zagreb part of the Organizing Committee would like to express our gratitude to the Ljubljana part of the Committee, and especially to V. Leban, for their effort in preparation of the meeting. Also, we experienced a very interesting trip, visiting a museum of the World war I and a fortress from the 19th century, during which we learned much about the history of this part of Slovenia.

And, counting the contributing authors (123 in total), I have found out that there are 15 authors, whose names begin with the letter B, 14 authors, whose names begin with M, and 13 authors, whose names begin with K. Last year Prof. Leban noticed at the end of the previous meeting, in his closing remarks, that the names starting with the letter P were the most common ones. P might stand for proteins. And this year, B may stand for biology, M for mineralogy, and K for kristalografija, as crystallography is spelled in Slovenian and Croatian languages.

The 14th Croatian-Slovenian Crystallographic Meeting will be held in the middle of June, in 2005, in Istria, Croatia, in a touristic resort at the Adriatic coast. We cordially invite all of you to attend the next meeting. We would also appeal to you to bring your friends and coworkers, at home or in other countries. Thank all of you very much and good luck until the next meeting in Croatia.

Unfortunately, one month later the region of Bovec and Kobarid was hit by an earthquake which caused substantial damage, but fortunately no human victims.

MEETING REPORT

EMC2

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El Jadida, Morocco, May 2004



About 130 crystallographers from North Africa and Europe gathered in May, 2004 for the 2nd Moroccan School of Crystallography, at the Faculty of Sciences campus of the U. Chouaib Doukkali of El Jadida. The IUCr was represented by its president, W. Duax. Organized by the U. of El Jadida and the Moroccan Crystallographic Assn (AMC) with the financial support of the IUCr, this 2nd school offered an opportunity for all Moroccan crystallographers and their foreign colleagues to get together and discuss their recent achievements. It was also a great opportunity for students to attend a high level conference and to discover different research areas of crystallography studied in Morocco and others countries, and to interact directly with teachers and researchers.



There were 15 lectures on various topics. The opening lecture on 'Crystallography and Nobel Prizes' was delivered by W. Duax (USA). Basic notions of crystallography as direct and reciprocal lattices and symmetry in crystals were presented by L. El Ammari and A. Thalal (Morocco). An application of the symmetry to Islamic art was given by E. Makovicky (Denmark).

A session was devoted to structural resolution. D. Avignant, E. Hlil, and P. Martinetto (France) presented structural studies of single crystals and powders. Complementary methods of structure solution using electron and neutron diffraction were given by R. Portier and M. Ann (Fance).

A. Durif (France) discussed the fundamentals of structural crystallography in the elaboration of the classification of phosphorus anions. We recall that Morocco is a great phosphate and phosphoric acid producer and a large number of crystallographers are leading research in this field. M. Pierrot and C. Lecomte (France) presented respectively crystallography of proteins and photocystallography of organic molecular materials. Using the Monte Carlo method to index powder patterns and solve structures was discussed by A. Le Bail (France). He also indicated how to access the public data bases and lab archives online. L. El Ammari, M. Saadi (Morocco) and E. Hlil (France) organized a practical session at which the students solved several structures by themselves.

One morning was reserved for the sponsors of the School to present new Rx instruments. The school finished with the bi-annual meeting of the members of the Moroccan Crystallographic Assn (MCA). The president and the treasurer presented the results of the activities of the last two years and the financial

state of the association.

On behalf of the MCA, I would like to thank the IUCr for taking an interest in our periodic crystallographic meeting and its financial support.

Abdelmalek Thalal

NOTICE

New President elected



Kazumasa Ohsumi

Kazumasa Ohsumi (KEK) was elected President of the Crystallographic Society of Japan (CrSJ) in April 2004. Other new members of the Executive Committee include: General Secretary: M. Takata (SPring-8); Treasurer: K. Sugiyama (U. of Tokyo); Chair of the Committee on Meeting and School of Crystallography: I. Nakai (Tokyo Science U.); Chair of the Committee on Public Relations: K. Tsuda (Tohoku U.); Chair of the Committee on Data Base and Information: H. Uekusa (Tokyo Inst. of Technology); Chair of the Committee on Journal of the CrSJ: N. Kamiya (RIKEN Harima).



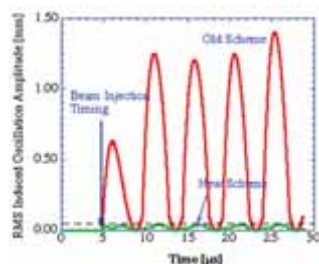
Tamaichi Ashida

Tamaichi Ashida, Professor Emeritus of Nagoya U., Japan, was elected as an Honorary Member of the Crystallographic Society of Japan (CrSJ) for his outstanding contribution to X-ray protein crystallography.

NOTICE

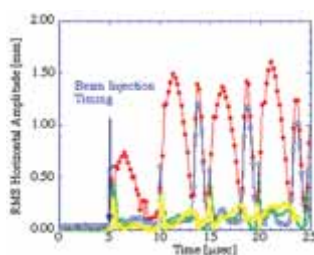
Top-up operation at SPring-8

Japan Synchrotron Radiation Research Institute (JASRI)



Simulation results of the stored beam oscillation induced in the horizontal plane by using the ideal half-sine field shape.

Accelerator Division (Director, Noritaka Kumagai) of JASRI (Director-General, Akira Kira) successfully started the top-up operation of the SPring-8 storage ring. In the top-up operation, beam is injected with short intervals during user beamtime, and the current stored in the storage ring is kept constant. In the conventional operation, on the other hand, the stored current decayed with time and during beam injections, user experiments were interrupted due to beam orbit instabilities. Therefore, we were hard-pressed to come up with improvement measures.



Experimental results for performance of the bump leakage suppression.

The top-up operation realized at SPring-8 provides the solutions to the above problems. Moreover, this operation has unique and innovative features such as (1) a perturbation-free beam injection scheme, (2) minimum injection beam loss, (3) a high purity singlebunch beam. The SPring-8 top-up operation is, in a sense, an 'ideal top-up operation' which many light source facilities around the world have pursued.

This success of the top-up operation is expected to make the following improvements: (1) The time-averaged brilliance is increased by a factor of two. (2) Thermal stability of the X-ray optics is attained by stabilizing the stored beam current with a deviation of less than 0.1%, and accuracy of experimental data is improved. (3) A new filling pattern with a high bunch current is made available, which was not available in the conventional operation due to the extremely short beam lifetime. This will pave the way for new SR experiments with intense pulsed X-ray. The top-up operation was introduced on May 20, 2004 to user beamtime and users have great hopes for this new operation.

For further information, visit the website www.spring8.or.jp/e/press/040618/top-up-e.html.

Kenji Tsuda

NOTICE

Australian Synchrotron

Two new contributors to the beamline pool have been announced: ANSTO and New Zealand.

The Minister for Innovation, J. Brumby, announced the Australian Nuclear Science and Technology Organization (ANSTO) would provide \$5 million toward initial beamlines planned for the Australian Synchrotron, which is on schedule and on budget. This commitment is in addition to \$15 million already committed by Melbourne U., Monash U., the CSIRO, and MiniFAB.

The Australian Synchrotron Research Program (ASRP), run out of ANSTO, offers researchers opportunities to use overseas synchrotrons, however, it is felt that a national facility is needed. Victoria's Premier, S. Bracks and New Zealand's Minister for Research, Science and Technology, P. Hodgson announced that New Zealand has agreed in principle to contribute AUD\$5 million towards the Australian Synchrotron beamlines. 'The Victorian Government has been bold and farsighted in committing to the capital cost of this crucial science infrastructure,' Mr. Hodgson said. 'New Zealand R&D will benefit substantially, and our in-principle commitment will give this nation a seat at the table in determining how the facility develops. 'Like Australia, New Zealand has so-called 'suitcase scientists' forced to go to the Northern Hemisphere to undertake leading edge R&D. This new Australian facility will bring the tools they need much closer.'

SCANZ Newsletter, No 58, August 2004

IUCR JOURNALS NEWS

IUCr pilots CrossRef Search



The IUCr is one of nine leading publishers to pilot CrossRef Search, a search facility that uses the collaborative environment of CrossRef combined with Google search technologies. Users can search the full text of high-quality peer-reviewed journal articles, conference proceedings and other resources. The pilot launches a typical Google search but filters the result set to the scholarly research content from participating publishers, with the intent of reducing the noise produced by general web searches. The other publishers taking part in this initiative are: American Physical Society, Annual Reviews, Association for Computing Machinery, Blackwell Publishing, Institute of Physics Publishing, Nature Publishing Group, Oxford University Press, and John Wiley & Sons.

The CrossRef Search pilot, which additional publishers are expected to join, will run through 2004 to evaluate functionality and gather feedback from scientists, scholars and librarians to fine-tune the program.

To use this free service or find out more information, please visit the search page of Crystallography Journals Online at <http://journals.iucr.org/services/search.html>.

OBITUARY

Sivaraj Ramaseshan (1923-2003)

An incurable romantic about science, Sivaraj Ramaseshan carried forward C.V. Raman's legacy. A fellow scientist pays his respects...

Sivaraj Ramaseshan, former Director of the Indian Inst. of Science and Professor-Emeritus at the Raman Research Inst., died in Bangalore on December 29, 2003. Born in 1923 at Nagpur, Ramaseshan had a career in science which stretched over half a century, during which he blazed a trail of original research and contributed enormously to the growth of many institutions of science in India.

Ramaseshan began his research career as a student under his legendary uncle, C.V. Raman. Following a Ph.D. in physics, he joined the faculty of the Indian Inst. of Science (IISc), Bangalore, as a lecturer. It was here that he established a vigorous school in the developing area of X-ray crystallography, in the 1950s. He returned to the institute in 1979 as its Joint Director, and later served as Director from 1981 to 1984. In the intervening period, Ramaseshan established the Physics Dept. at the Indian Inst. of Technology, Madras, and the Materials Science Div. at the National Aeronautical Laboratory (NAL). At NAL, Ramaseshan led a world class program which has proved critically important in the development of materials research in India. Optics, crystallography, and high pressure physics were areas where Ramaseshan made decisive and influential contributions, which were recognized by several national awards including the Padma Bhushan.

Ramaseshan was far more than a researcher lost in the technicalities of his chosen discipline. He was a builder of groups, institutions, scientific organizations, and academies. He was the prime architect of a movement to enhance the visibility, prestige, and content of science journals published from India. He was among the foremost popularizers of science in this country. To every sphere of his diverse activities Ramaseshan made distinctive and lasting contributions.

In 1984, when he formally retired from his position as the Director, IISc, he began a remarkable post-retirement phase, returning to a routine of research, seminars, writing, and lecturing.

In 1989, he took over the editorship of Current Science. This journal, founded in 1932, had an illustrious past but had fallen on hard times, with diminishing circulation and visibility. He brought to the task of rejuvenating Current Science, a remarkable sense of purpose and boundless optimism, succeeding in his

task, before failing health began to take its toll.

When C.V. Raman died in 1970, he left three institutions: the Raman Research Inst., the Indian Academy of Sciences, and the Current Science Association, all of which he had presided over for long periods of time. In the years that followed, Ramaseshan, more than anyone else, tended to the Raman legacy, ensuring that these organizations acquired a new and distinctive character. He served on their councils and governing bodies for long periods of time, devoting considerable effort towards their welfare. He served as the President of the Indian Academy of Sciences between 1983 and 1985.

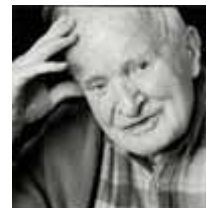
In reflecting on the life and times of Ramaseshan, we must also remember his great contemporaries, G.N. Ramachandran (1922-2001) and Satish Dhawan (1920-2002). For a brief period, in the transition years between the 1970s and 1980s, all three were at IISc. They were three entirely different personalities, but they all bore the indelible stamp of greatness, contributing substantially to the growth of our science and our institutions. With Ramachandran, Ramaseshan shared a deep and abiding interest in optics and crystallography. With Dhawan, he shared a total commitment to building and fostering the institutions on which this country's progress depends.

Ramaseshan was incurably romantic about science. In 1978, delivering the first C.V. Raman Memorial Lecture at IISc, he recalled: 'To Raman, scientific activity was the fulfillment of an inner need. His approach to science was one of passion, curiosity, and simplicity. It was an attempt to understand. To him science was based on independent thought, combined with hard work. Science was a personal endeavor, an aesthetic pursuit, and above all, a joyous experience.' In full measure, these words also describe Ramaseshan's approach to science. He was an outstanding lecturer and conversationalist. His self-deprecatory humor and ability to laugh at himself were engaging. Sivaraj Ramaseshan lived a full life, contributing greatly to his surroundings. Those who knew him personally were immeasurably enriched. In his death, science in India has lost one of its most distinguished practitioners.

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OBITUARY

Arthur R. von Hippel (1898-2003)



MIT Institute Prof. Emeritus Arthur Robert von Hippel, who fled to the USA from Nazi Germany and went on to become a leader in materials research, died on December 31. He was 105 years old.

His name graces the highest international honor awarded in his field. The von Hippel Award of the Materials Research Society has been presented annually since 1976; von Hippel himself was the first recipient.

Although not a crystallographer himself, von Hippel inspired many crystallographers in the field of materials science, including four who came through his lab, subsequently becoming presidents of ACA: Rob Burbank, Howard Evans, Bob Newnham, and Sidney Abrahams.

His son, Eric von Hippel, said his father cross-country skied until he was 95 and continued to exercise by walking a mile a day even into his 100s.

*From Obituary published by MIT
January 2004*