

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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Original article text and available illustrations

Contents

Letter from the President

Letter from the President	4
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Letter to the Editor

Letter to the editor	6
Tilting at windmills	7

Editorial

Letter from the Editor	8
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IUCr journals news

Ab initio structure solution by charge flipping. II. Use of weak reflections	9
Remarkable features in lattice-parameter ratios of crystals. I. Orthorhombic, tetragonal and hexagonal crystals; II. Monoclinic and triclinic crystals	10
Pseudomerohedrally twinned crystal structure of 2,3-diphenylbuta-1,3-diene	11
The endoproteinase furin contains two essential Ca ²⁺ ions stabilizing its N-terminus and the unique S1-specificity pocket	12
Chloropyridinebis[tricarbonyl(η 5-cyclopentadienyl)-tungstenio]indium	13
Structural analysis of caspase-1 inhibitors derived from Tethering	14
The derivation of the cellulose microfibril angle by small-angle X-ray scattering from structurally characterized softwood cell-wall populations	15
Synchrotron radiation and high pressure: new light on materials under extreme conditions	16

Special report

Overview of crystallography in Japan (1913 – 1980)	17
--	----

Feature article

Yuji Ohashi	28
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Meeting report

2004 annual meeting	29
2005 annual meeting of JSSRR	31
Crystal growth under Popocatepetl	33
MaThCryst 2005	35
Recent advances in X-ray powder diffraction	36

Awards and prizes

Bricogne receives honorary doctorate	37
2005 Art in crystallography winners	38
Academy membership for Alexander Wlodawer	39
Jones receives Patterson Award	40
ACA announces 2006 Buerger and Warren Award winners	41
 Notice	
Announcements	42
 Obituary	
Lyudmila Gorogotskaya (1935–2005)	43
Mary Rosaleen Truter (1925–2004)	44

LETTER FROM THE PRESIDENT

Letter from the President



W.L. Duax

A principle goal of the IUCr is to nurture leadership in all areas of crystallography in all countries of the world. Women have played a major role in the growth and development of crystallography throughout its history and make up a significant part of the crystallographic community in all member countries. Nevertheless, there appears to be a significant underrepresentation by women in the composition of National Committees, the delegates to the General Assembly, the recommendations made by the National Committees for membership on the Commissions of the IUCr, the resulting composition of the Commissions and the individuals proposed by Commission to represent their interests on the Program Committee for the 2008 IUCr Congress in Japan. In the best interest of crystallography, we must see to it that women are represented on National Committees and IUCr Commissions in proportion to their population in the crystallographic community. Furthermore, in Countries or Commissions where participation by women is low or nonexistent, it is essential that measures be taken to see to it, that there are no impediments to female participation and that women be encouraged to participate. The chairs of the 15 Commissions of the IUCr were asked to identify their probable successors and propose the composition of their Commissions for 2005 - 2008. There was a conspicuous absence of women's names on the early responses. Consequently, I urged all Commissions to strive for equitable representation by women. I also asked Commission Chairs to recommend at least two nominees for the Program Committee for Osaka, one of which should be female. Some Commissions responded that they were hampered in achieving gender balance because they only consider nominations from National Committees and none of the National Committees had nominated any women for their Commissions. Because the expertise of the members of a Commission is greater than that of the National Committee in their topic areas I urge them not to be limited in their nomination to input from National Committees.

In May, 2005 the secretaries of all National Committees were asked for information about the history, structure and composition of their National Committees, information about any National Crystallographic Association in their country, the names of the delegates they would be sending to the Congress in Florence, and the name of the guest editor for the special issue of the IUCr devoted to their country. There are no women on nine of the 23 National Committee in countries that responded and no women officers in five of the 14 National Crystallographic Associations for which data were provided. The ratio of male to female coeditors of IUCr Journals is 116 to 18 and two of the journals have no women editors.

In order to obtain reliable data concerning the ratio of women to men in our community upon which to assure equitable access to positions of leadership we need statistics on the distribution of males and females in National Crystallographic Associations, attendees at national and international meetings and student applications for financial support to attend meetings supported in part by the IUCr. In order to help National Committees and IUCr Commission Chairs to identify women who are qualified and interested in participating in the work of the vital committees, I wish to create a website of women volunteers. I invite all women crystallographers to register on this website with a short biography covering their areas of expertise and listing not more than three recent representative publications. Send the information to me or to the IUCr newsletter office so that we can build this important database. I welcome any advice and suggestions with respect to data and format for the database.

The IUCr President's Discretionary Fund has often been used to help senior scientists from disadvantaged countries to attend IUCr Congresses. Unfortunately information about the existence and use of this fund has not been uniformly available to all crystallographers or the National Committees of all member countries. Requests for assistance to attend the Congress in Florence were addressed to Mike Dacombe, the Executive Secretary, to Carlo Mealli, the Program Chair for Florence, and to me. There were over 40 requests for assistance to attend the Florence meeting with as many as seven coming from the same country. The distribution of awards by country was one each in Armenia, Bangladesh, Czech Republic, Colombia, Cuba, India, Israel, Romania, South Africa, Turkey, and Uzbekistan, two each in Argentina, Croatia, and Ukraine, and four in Russia.

The gender distribution of the requests was not balanced and only four awards went to women. Mike and I would like to establish guidelines for future use of the President's Fund to support attendance to IUCr Congresses by senior scientists. In addition to a formal request, the applicant should have letters of support from a Regional Affiliate of the IUCr and if possible from a National Committee, a short CV and one representative publication. In the future we may ask Regional Affiliates to rank the applicants from their region. The same individual should not be eligible to receive support from the President's Fund twice in a six-year period.

Bill Duax, duax@hwi.buffalol.edu

LETTER TO THE EDITOR

Letter to the editor

Dear Judy,

I missed the letter or article that stimulated a cluster of reminiscences in the latest issue of the newsletter concerning the late Prof. Belov. But on his visit to the UK in 1960, he visited Aberdeen and stayed with us as a house guest. At one point during his visit, he announced himself unwell and liable to coronary failure. Concerned with our responsibility for such a distinguished visitor, we immediately (this was 1960!) arranged an appointment for him with our practitioner. We explained the situation over the phone and our doctors rose to the occasion: Belov was seen by the most senior partner. I was asked to stay during the examination in case assistance was needed with translation. It quickly emerged that Belov was taking the latest German medicines -at that time reserved for a favoured few- and had made an in-depth clinical study of his condition. In fact, his "emergency" was concocted as he really only wanted to find out if there were better British medicines/treatments available; the "examination" rapidly turned into a general discussion of his (Belov's) condition and options for its management. So charmed was our doctor (and Belov could really charm an audience) that they spent over an hour together with the conversation ranging widely.

Fred Glasser

Dear Fred,

Thanks so much for this charming story.

Judy

LETTER TO THE EDITOR

Tilting at windmills



In 1961 Kathleen Lonsdale and Judith Milledge, *Acta Cryst.* (1961). **14**, 59-61, published a paper entitled "Analysis of thermal vibrations in crystals: a warning". I was a referee for that paper. In my report, I said that Lonsdale and Milledge had somewhat misrepresented the papers they were criticising and "were tilting at windmills of their own creation". In her response, Lonsdale denied my charge and enclosed a charming figure, reproduced here, showing "The authors tilting at a windmill". Note the self-portraits, and the offenders named on the sails. Recently I showed this to Bill Duax, who felt it should be shared with a wider audience and no longer kept under "a veil of referral anonymity." My reports evidently had some effect, for in publication Lonsdale and Milledge concluded graciously "We should like to acknowledge our indebtedness to the referee whose sharp criticisms made us re-write this paper and, we hope, improve it".

Kathleen Lonsdale (1903-1971) began her long career in X-ray crystallography under W. H. Bragg in 1922. In 1929 she determined the structure of hexamethylbenzene, the first aromatic compound to be defined by X-ray diffraction, and so proved the planarity of the benzene nucleus. She was a pioneer of space group theory in relation to the structure analysis of crystals and was an indefatigable editor of *International Tables* for many years. Among other fields she was an expert on thermal diffuse scattering, divergent beam X-ray photography and synthetic diamonds. At the Moscow Congress in 1966 she became President of the IUCr. Dorothy Hodgkin wrote in her obituary "She was a tough president, who kept her committees working for long hours. Professor Belov, who succeeded her as President, was heard to remark as she dragged him away from a pleasant party at the British Embassy to yet another committee meeting: 'Kathleen you are a martinet'".

Durward Cruickshank

EDITORIAL

Letter from the Editor



This issue of the Newsletter contains the first set of articles highlighting Crystallography in Japan. Japan is the fourth geographical area to be covered in our series 'Crystallography Around the World'. The series started off with Crystallography in Latin America (Volume 11, Number 3, 2003) and was followed by Crystallography in Italy (Volume 12, Number 1, 2004, and then Crystallography in Russia (Volume 12, Numbers 2 and 4, 2004). Already on hand in the editorial office are articles on Crystallography in Portugal and in the Pacific Rim region of Australia and New Zealand and several others are planned. We hope that you have been enjoying these articles and invite you to suggest areas of the globe that you would like to see covered in future issues.

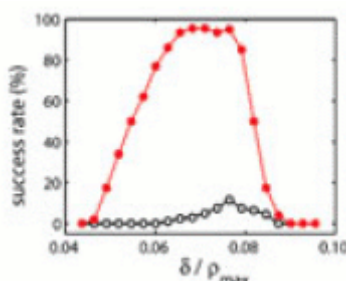
Starting with the next issue (Volume 13, Number 3) we will be presenting extensive coverage of the IUCr Congress in Florence. This coverage will most likely be spread over at least three issues of the Newsletter so be patient if the review for your session does not appear in the first set.

Each issue of the Newsletter also contains editorials, meeting reviews, news of crystallographers and a calendar of upcoming meetings. Our readers are the best source of information for these articles so please continue to send them and to be on the lookout for items you think would be of interest to our crystallographic family. I would also welcome 'letters to the editor' with your comments on the Newsletter itself, the world condition as it affects crystallography, reminiscences, suggestions, etc. By the time you see this the Florence Congress will be over and we will be hard at work preparing the first issue containing the meeting reviews. Thanks to all of you who stopped by to say hello to Patti at the IUCr booth during the Congress exhibition and please do keep in touch.

Judy Flippen-Anderson
flippen@rcsb.rutgers.edu

Ab initio structure solution by charge flipping. II. Use of weak reflections

Acta Cryst. (2005). **A61**, 147-152



Success rates for a hard-to-solve structure of the original and new charge flipping algorithms (black and red symbols).

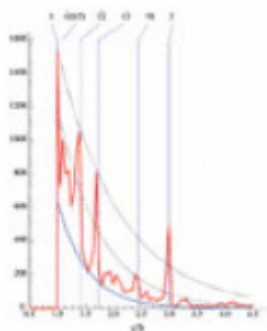
Charge flipping is an amazingly simple iterative algorithm that is based on extended zero regions of the electron density, but not directly on atomicity. In the original version [Oszlányi & Sütő (2004). *Acta Cryst.* **A60**, 134-141] the phase space was explored by changing the sign of electron density below a threshold δ . This process can be efficiently improved in reciprocal space by handling weak reflections in a special way: their calculated moduli are allowed to change freely and calculated phases are shifted by $\pi/2$.

Paradoxically, using less observed data as constraints allows the solution of larger structures.

Gábor Oszlányi and András Sütő

Remarkable features in lattice-parameter ratios of crystals. I. Orthorhombic, tetragonal and hexagonal crystals; II. Monoclinic and triclinic crystals

Acta Cryst. (2005). B61, 287-295; 296-303



Frequency distribution of orthorhombic inorganic crystals as a function of c/b (in red). All important peaks correspond to integral lattices.

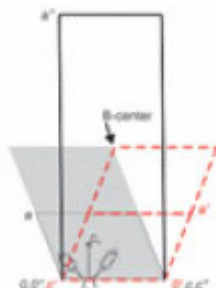
The basic features of frequency distribution as a function of lattice-parameter ratios are reported.

Observed are exponential decay evidenced by increasing ratios and sharp peaks, possibly due to integral lattices, with one of the most important peaks at the ratio 1:1. Most of these features do not follow from classical crystallographic principles. Some of these properties can be interpreted on the basis of a general crystallography, where crystallographic scaling is considered. These results are compatible with crystallographic properties observed in a number of axial-symmetric proteins.

R. de Gelder and A. Janner

Pseudomerohedrally twinned crystal structure of 2,3-diphenylbuta-1,3-diene

***Acta Cryst.* (2005). C61, o300–o302**



Orientation of the molecule in the monoclinic crystal lattice and its relation to the *B*-centered pseudo-orthorhombic twin lattice.

This article describes the structure determination of the small organic molecule $C_{16}H_{14}$ and a proposed nano-scale twinning model. The monoclinic crystal lattice is twinned by reticular pseudomerohedry (index 2) to form a *B*-centered orthorhombic supercell (twincell) with $\beta = 90.6^\circ$. The approximate molecular twofold axis coincides with the twin axis and a lattice direction of the supercell. This paper illustrates that currently available twin-detection software (*Dirax*, *Rotax*, *PLATON**TwinRotMat*), twin-integration software (*EvalCCD*) and twin-refinement software (*SHELXL*) can make a previously involved problem routine.

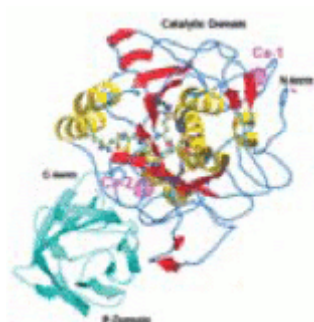
M. Lutz, A. L. Spek, B. C. van der Wiel and C. A. van Walree

IUCR JOURNALS NEWS

The endoproteinase furin contains two essential Ca^{2+} ions stabilizing its N-terminus and the unique S1-specificity pocket

The endoproteinase furin contains two essential Ca^{2+} ions stabilizing its N-terminus and the unique S1-specificity pocket

Acta Cryst. (2005). D61, 505-512



Ribbon plot of furin (yellow helices and red β -strands for the catalytic domain, P-domain entirely in cyan) together with the calcium-specific double difference Fourier map ('difference DANO map' in purple).

We have unequivocally determined the exact number and the three-dimensional localization of essential calcium sites within furin, a calcium-dependent endoproteinase of the prohormone/proprotein convertase (PC) family, employing a novel type of double difference Fourier map. This 'difference DANO map' was calculated from complete anomalous diffraction data collected on either side of the calcium K absorption edge in the softer X-ray regime and can also be applied to the unambiguous determination of all elements, for which an absorption edge can be accessed for diffraction experiments.

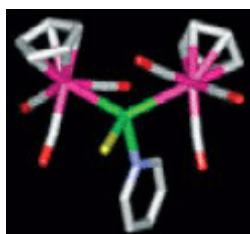
Manuel E. Than, Stefan Henrich, Gleb P. Bourenkov, Hans D. Bartunik, Robert Huber and Wolfram Bode

IUCR JOURNALS NEWS

Chloropyridinebis[tricarbonyl(η^5 -cyclopentadienyl)-tungstenio]indium

Chloropyridinebis[tricarbonyl(η^5 -cyclopentadienyl)-tungstenio]indium

h2>Acta Cryst. (2005). E61, m945–m946



The structure of $\text{In}\{\text{W}(\text{C}_5\text{H}_5)(\text{CO})_3\}_2\text{-(C}_5\text{H}_5\text{N)Cl}$ (In: green, W: pink, Cl: yellow, N: blue, C: gray, O: red). Only three crystal structures have been reported to date for indium complexes with In–W bond(s), and there is no X-ray structure for an indium-bridged ditungsten complex. The title complex is the first crystal structure of such a complex. The complex was prepared from InCl_3 and 2 equivalents of $\text{K}[\text{Cp}(\text{CO})_3\text{W}]$ followed by the addition of pyridine. The X-ray analysis revealed that the In atom has Cl and pyridine substituents and bridges two $\text{Cp}(\text{CO})_3\text{W}$ fragments, resulting in a distorted tetrahedral geometry around the In atom.

H. Nakazawa, M. Itazaki and M. Owaribe

Structural analysis of caspase-1 inhibitors derived from Tethering

***Acta Cryst.* (2005). F61, 451-458**



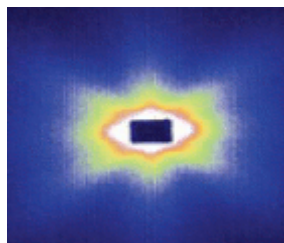
Crystal structure of caspase-1 covalently modified with the extender. Hydrogen bonds between the extender and the protein are displayed as dashed yellow lines with their associated distances shown in black. Selected residues comprising the active site are also shown.

A fragment-assembly approach, accompanied by structural analysis, was employed to generate caspase-1 inhibitors with cell-based activity. With the aid of Tethering® with extenders (small molecules that bind to the active-site cysteine and contain a free thiol), two novel fragments that bound to the active site and made a disulfide bond with the extender were identified by mass spectrometry. Direct linking of each fragment to the extender generated submicromolar, reversible inhibitors that significantly reduced secretion of the caspase-1-processed cytokine interleukin-1 β from human peripheral blood mononuclear cells.

T. O'Brien, B. T. Fahr, M. M. Sopko, J. W. Lam, N. D. Waal, B. C. Raimundo, H. E. Purkey, P. Pham and M. J. Romanowski

The derivation of the cellulose microfibril angle by small-angle X-ray scattering from structurally characterized softwood cell-wall populations

J. Appl. Cryst. (2005). 38, 505-511



A small-angle scattering pattern for a wood specimen with the X-ray beam directed normal to the radial plane.

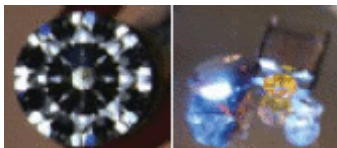
The micro-fibril angle M of the cellulose helices in the S_2 layers of the cell walls of softwood has been measured. The values were obtained by fitting the calculated azimuthal distribution of small-angle scattered X-ray intensity to the measured distribution. The calculated distribution was obtained by measuring the width and the orientation of over 100 cell walls in the irradiated volume and summing the intensity scattered by them. Values of M obtained using six different orientations of the specimen in the X-ray beam showed good agreement. Errors arising from the frequently made assumption that the cells are rectangular have been established.

K. M. Entwistle, S. J. Eichhorn and N. Navaranjan

IUCR JOURNALS NEWS

Synchrotron radiation and high pressure: new light on materials under extreme conditions

J. Synchrotron Rad. (2005). **12**, 135-154



Single-crystal diamonds grown by chemical vapor deposition being used in a new generation of high-pressure synchrotron studies of materials under extreme conditions.

Recent diamond-anvil cell experiments using new synchrotron X-ray and infrared techniques are revealing a wealth of phenomena in materials up to multimegabar pressures. Significant advances have occurred in high-pressure powder and single-crystal diffraction, spectroscopy, inelastic scattering, radiography, and infrared spectroscopy of simple molecular systems such as hydrogen, novel high-pressure metals and superconductors, high-density minerals, glasses and liquids, as well as biomolecules under extreme conditions. As such, the findings have implications for problems that span physics, chemistry, materials science, geoscience, planetary science, and biology.

R. J. Hemley, H.-K. Mao and V. V. Struzhkin

SPECIAL REPORT

Overview of crystallography in Japan (1913 - 1980)

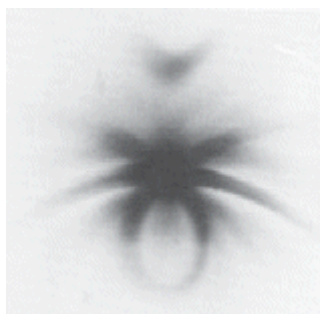
Modern crystallography in Japan started right after Laue's discovery of diffraction of X-rays by crystals (1912), and many valuable achievements were realized during those early years. To our regret, most of them were not recognized outside of Japan. This article will present an outline of crystallography in Japan, especially crystal structure determination, from its advent to approximately 1980. The reviewer apologizes that he cannot fully review research in physics and mineralogy since he is a chemist.

The early years of Crystallography to about 1945



Prof. S. Nishikawa

In 1913, T. Terada tried X-ray experiments using a rock salt crystal and a fluorescent screen in a dark room. He observed several diffraction spots and that they moved according to the movement of the crystal. He explained this phenomenon as reflection of the incident X-ray beam from the atomic net planes in the crystal (*Nature* **91**, 135 (1913)). His work paralleled that reported by Bragg (*Nature* **91**, 557 (1913)).



Laue photograph of asbestos fiber, the fiber axis inclined 45° to X-ray beam, Pt white X-ray (September, 19, 1913) (Nishikawa, S. and Ono, S., *Proc. Math. Phys. Soc. Tokyo*, **7**, 131 (1913)).

S. Nishikawa, stimulated by Terada's experiment, began X-ray diffraction studies with Pt white X-rays of (i) fibrous materials such as cotton, silk, and asbestos, (ii) minerals such as mica and talc, and (iii) crystalline powders of fluorite and zinc blende. He found that materials of group (i) were aggregates of micro crystals having a common (fiber) axis, group (ii) were stacked aggregates of thin leafy crystals, and group (iii) were randomly oriented powdered crystals (*Proc. Math. Phys. Soc. Tokyo*, **7**, 131 (1913)). He was a pioneer in the area of X-ray studies of structures of complex compounds. Nishikawa (1915) then studied the structure of spinel, using Laue photographs with space group theory. This was the first case in which space group theory was applied to crystal structure determination. Nishikawa and K. Matsukawa (1928) verified, by experiments on zinc blende, the breakdown of Friedel's law for crystals containing atoms which anomalously dispersed incident X-rays. This work was reported two years earlier than that of Coster, Knol, and Prins (1930).



Prof. I. Nitta

In 1922, Nishikawa organized a crystallography research group that used both X-ray and electron diffraction in the Institute for Physical and Chemical Research (Tokyo). I. Nitta, a member of the group, studied the crystal structure of pentaerythritol $C(CH_2OH)_4$ to establish tetrahedral carbon valence bonds. At that time, however, there was a report based on a space group assignment that the central C atom of pentaerythritol in the crystal was (tetragonal) pyramidal. Nitta (1926) found that the reported space group was erroneous and the C atom was actually tetrahedral. This was later verified by a full structure determination, and the tetrahedral carbon valence bonds were established. Nitta served as Vice President of IUCr from 1963 to 1969.



T. Ito

S. Kikuchi, a member of Nishikawa's group, began research on electron diffraction right after the experiments by Davisson, Germer and Thomson in 1927. Kikuchi then succeeded in doing high-energy electron diffraction (HEED) studies on single crystals of mica (1928). He observed several characteristic features of HEED, now known as the Kikuchi pattern. Several crystallographers in this group, S. Miyake, R. Uyeda, N. Kato and others studied the diffraction physics of both X-rays and electrons.

In 1924 T. Ito, who studied crystallography with P. Niggli and later with W. L. Bragg, organized a research group on mineralogical crystallography at the Univ. of Tokyo. In 1933, Nitta organized a crystallographic research group at Osaka Univ.

(1945 - 1980)

Diffraction physics : N. Kato experimentally and theoretically studied X-ray dynamical diffraction, section topographs and secondary extinction. He was President of IUCr (1978~1981), and a winner of the IUCr Ewald Prize. K. Kohra was the principal crystallographer working on the construction of the Tsukuba Photon Factory, which is still one of the most productive SR sources in the world.

Mineralogical crystallography: from 1945 - 1955 T. Ito and his collaborators, R. Sadanaga, Y. Takeuchi, N. Morimoto and others, determined crystal structures of important minerals. Ito developed a powerful indexing method for X-ray powder diffraction patterns, the Ito method. During this period, Ito established the general idea of 'cell twin' or 'Ito twin' for 'repeated twinning of unit cell level'. This twin was quite different from the macroscopic one. These results were published in *X-ray Studies on Polymorphism* (Maruzen, 1950).

Sadanaga and others systematized Ito's theory of the twin space group. Takeuchi studied the crystal structures of minerals under high pressure and/or high temperature. Morimoto, M. Tokonami and Y. Koto studied structures, superstructures and phase-transitions of many minerals.

Instruments: One of the first large computers built in Japan, comparable to IBM systems, that had enough capacity for computing in crystal structure determination came into operation in 1967. A program system UNICS (universal crystallographic computing system) consisting of fundamental programs for structure determination was written by T. Sakurai, T. Ashida and others (1967), and used by many crystallographers. The first Japanese computer-controlled four-circle diffractometer was produced

in 1968 by Rigaku. Then the precision as well as the speed of X-ray single crystal structure determination in Japan improved dramatically. Tsukuba photon factory 2.5GeV came into operation in 1983. It provided a large step forward for the development of crystallography in Japan which saw an ensuing growth in the number of researchers involved in structure determination.

Anomalous dispersion: Using anomalous dispersion Y. Saito and collaborators (1954) were among the first to determine absolute configuration with their work on the complex ion $[\text{Co(en)}_3]^{3+}$. Y. Okaya, Saito and R. Pepinsky proposed the theoretically attractive $Ps(u)$ function. Okaya and Pepinsky formulated the relationship between structure factor phases and anomalous dispersion terms. This relationship is used in the phasing method which is now most widely applied for protein crystallography.

Electron density distribution: Y. Tomiie *et al.* (1958) studied precise electron density distribution in diformylhydrazine and obtained a reasonable coincidence with the one calculated by the MO method. He also found the electron density of a lone pair of electrons belonging to the O atom. Saito, F. Marumo and others studied precise 3d electron distribution in some transition metal ions and compared their results with theoretical predictions. Saito, H. Iwasaki and others studied electron density distributions in charge transfer complexes.

Important compounds: Crystal structures of many important compounds, such as natural organic compounds, coordination compounds, organometallics (A. Shimada, N. Kasai and N. Yasuoka), charge transfer complexes, synthetic polymers (H. Tadokoro), oligopeptides (Ashida), etc, have been studied. Many crystallographers are engaged in research in this category, but only a few of them could be presented here for want of space.

Crystalline phase reactions : In 1977, Y. Ohashi and Y. Sasada observed that racemization occurred when crystals of an (S- α -methylbenzylamine)cobaloxime complex were exposed to X-rays. This reaction could be traced by observing changes in electron density with exposure time. Similar reactions were found in the crystals of related compounds and were extensively studied. This research exploited a new attractive research field in chemical crystallography.

Protein crystals: M. Kakudo, Ashida, N. Tanaka and others began protein crystallography in 1965, and reported a 2.3 Å resolution structure of bonito ferrocycytochrome c at the IUCr meeting in 1972. Most of the MIR programs necessary were prepared by Ashida. This was the first high-resolution analysis of a protein structure in Japan. In an international collaboration involving the staff of Dorothy Hodgkin's laboratory in England, N. Sakabe and others studied 2Zn-insulin at 3.1 Å resolution in 1972 and 1.1 Å resolution in 1984. Y. Iitaka and Y. Mitsui and others studied 2.6 Å resolution subtilisin inhibitor in 1979. Katsube's group reported the structure of ferredoxin in 1981. From that point on protein crystallography in Japan developed rapidly in both quality and quantity.

Other biological materials: DNA, RNA and related compounds were studied by Y. Mitsui and Iitaka, Sasada's group and K. Tomita's group. Bacterial cilia and flagella, muscle, biomembranes, etc have been studied. Among many biophysicists who engaged in the research of these material were T. Mitsui's group including T. Ueki, and K. Wakabayashi.

Crystallographic community



50th Anniversary Celebration. (left to right) Y. Fujii (Chair of NCC-Japan, Program Chair of IUCr2008); F. Iwasaki (President of CrSJ); late N. Kato (the former IUCr President, 1978-1981); M. Tanaka (Vice President of IUCr); Y. Ohashi (President of AsCA, EC member of IUCr)

Japan joined the IUCr in 1951 with its adhering body being the National Committee for Crystallography (NCC-Japan), which adheres to the Science Council of Japan (SCJ). The Crystallographic Society of Japan (CrSJ) was organized in 1950 as the electorate for the national committee. The number of members is now about 1,300. CrSJ has held annual meetings since 1973, and has published the *Journal of the Crystallographic Society of Japan* (bimonthly) since 1960.

The Japanese crystallographic community has hosted several successful international meetings including the IXth Congress and General Assembly of the IUCr, Kyoto (1972), the 7th Sagamore Conference, Nikko (1982) and the International Summer School on Crystallographic Computing, Kyoto (1983)

CrSJ and NCC-Japan jointly celebrated the 50th anniversary of crystallography in Japan in Tokyo on July 1, 2000.

Tamaichi Ashida

(ashida-t@mpd.biglobe.ne.jp)

Activities in big facilities

SPring-8



SPring-8, the largest third-generation synchrotron radiation facility in the world, provides the most powerful synchrotron radiation currently available. The Japanese Atomic Energy Research Institute (JAERI) and RIKEN (The Institute of Physical and Chemical Research) began constructing SPring-8 (Super Photon ring-8GeV) in 1991 with support from Hyogo Prefecture, universities, research institutes and industries, and opened the facility in October, 1997.

Since its completion, all aspects of its operation have been conducted by the Japan Synchrotron Radiation Research Institute (JASRI), which was designated as the sole institute for the management, operation and development of SPring-8. SPring-8 consists of a 1GeV linear accelerator and 8GeV booster synchrotron that generates an incident electron beam of 8GeV and a storage ring (electron energy, 8GeV; current, 100mA; circumference, 1436m) that holds the generated electrons. Figure 3-1-1 shows the Bird's-eye view of SPring-8.

There are two types of light sources in SPring-8, insertion devices and bending magnets. Insertion devices are either undulators or wigglers. SPring-8 beam ports include insertion device beamlines with a 6m straight section (max. 34, existing 26), long insertion device beamlines with a 30m long straight section (max. 4, existing 1) and bending magnet beamlines (max. 24, existing 21). In-vacuum type undulators developed at SPring-8 have magnet arrays sealed in a vacuum chamber. The arrangement

results in a smaller gap between arrays, allowing radiation with shorter wavelength and higher power to be generated.

There is an in-vacuum revolver variable polarization undulator, an in-vacuum figure-8 undulator, a twin helical undulator, a tandem vertical undulator, an elliptical wiggler, and others that generate a variety of polarized radiation. The characteristic photon energy of a bending magnet is 28.9 keV.

62 beamlines are available. 46 are in operation and 2 are under construction. The beamlines are classified as public beamlines, contract beamlines, JAERI/RIKEN beamlines, R&D beamlines, and beamlines for accelerator diagnosis.

Two beamlines, whose lengths are 225m, are already operational at the biomedical imaging center. Two beamlines, longer than 100m, have been developed at the RI laboratory for research on radioactive isotopes and actinide materials. A 1 km-long beamline is used for research on advanced coherent X-ray optics.

The top-up operation was started successfully at SPring-8 in May, 2004. The electron beam is injected at short intervals during user beamtime, so that the current stored in the storage ring is kept constant. The top-up operation has a number of innovative features such as (1) a perturbation-free beam injection scheme, (2) minimum injection beam loss, and (3) a high purity singlebunch beam. This “ideal top-up operation” is used by many other light source facilities around the world. The top-up operation offers the following benefits to users: (1) time averaged brilliance is increased by a factor of two, (2) improvement of thermal stability of the X-ray optics, and (3) a new filling pattern with a high bunch current that was not available in more conventional operations due to the extremely short beam life-time.

SPring-8 invites proprietary and non-proprietary research proposals in June and November and does not charge users for beam time if their research is non-proprietary. The annual operation time of Spring-8 is around 5400 hours, with more than 4200 hours available for experiments. More than 1000 research subjects are accepted annually by SPring-8, and the number of researchers involved exceeds 10000.

Hideo Ohno, SPring-8

Photon factory

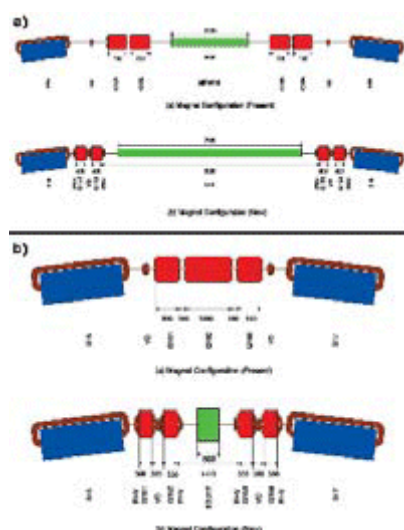


Fig. 3-2-1. Modification of Q-magnet arrangement for the straight section upgrade of the 2.5 GeV ring. (a) Lengthening existing straight sections. (b) Creating new straight sections.

The Photon Factory was the first synchrotron radiation research facility for X-rays in Japan. It operates two electron storage rings, shown in Table 1. One is a 2.5 GeV ring that has been operational since 1982. Its emittance was 400 nm·rad in the beginning, but was reduced to 36 nm·rad with upgrades in 1986 and 1997. The other is a single bunch operated 6.5 GeV electron storage ring which had been used

parasitically since 1986 and then in dedicated mode for synchrotron radiation research since 1997. This ring has a unique feature that 100 ps wide X-ray pulses are always obtained with a repeat period of 1.24 micro seconds. There are currently 7 and 4 insertion device beamlines on the 2.5 GeV and 6.5 GeV rings, respectively. The BL-2 of the 2.5 GeV ring is a soft X-ray undulator beamline which was the first in Japan and the second in the world. There are two in-vacuum undulator beamlines on the 6.5 GeV ring one of which is the first in-vacuum undulator beamline in the world and has been used extensively for the study of nuclear Bragg scattering, which makes the best use of pulsed X-Rays. A new in-vacuum X-ray undulator beamline is under construction on the 6.5 GeV ring for the study of photo-induced phase transitions in highly correlated materials.

There are 32 X-ray experimental stations out of 58 on the 2.5 GeV ring (energy ranging from 2.2 to 100 keV) and 8 X-ray experimental stations out of 9 on the 6.5 GeV rings (energy ranging from 5 to 160 keV). Among those 40 X-ray stations, 22 are for non-biological diffraction/scattering experiments, 5 for protein crystal structure analysis, 2 for small angle scattering, 8 for X-ray spectroscopy, 2 for X-ray imaging and 2 for others. There are 650-700 active experimental proposals every year and approximately 2,700 users repeatedly visit the Photon Factory to carry out their experiments. Eighty to eighty-five percent of proposals are for X-ray experiments, the others are for VUV/soft X-ray experiments. Since the inauguration of the facility in 1982, a number of contributions have been made at the Photon Factory. Those are, for example, MAD analysis of protein crystal structures using synchrotron radiation data, extensive use of image plates for X-ray diffraction experiments, development and extensive use of multi-anvil cells for structure studies under high pressure and high temperature, development of an X-ray Fresnel lens, experimental studies of resonant magnetic X-ray scattering, development of a quarter wave X-ray phase plate using a Bragg-transmitted beam, use of anomalous scattering methods for the study of orbital order in crystals, the development of an in-vacuum undulator and its extensive use for the study of nuclear Bragg scattering, and extensive use of a high energy X-ray elliptical wiggler for magnetic Compton scattering.

To meet requests for more experimental opportunities on insertion device beamlines, the lattice of the 2.5 GeV ring will be modified in the summer of 2005 to increase the number of straight sections for insertion devices. The modifications place new quadrupole magnets of shorter length with higher field gradients closer to neighboring bending magnets to lengthen the existing straight sections or to create new straight sections as shown in Fig. 3-2-1. Four short straight sections of 1.5 m will be created. Furthermore, two 5 m long straight sections will be lengthened to 9.2 m, and 8 other sections of 3.5 m will become more than 5 m. Except for one straight section used for electron beam injection, a total of 13 straight sections will be available for insertion devices on the 2.5 GeV ring. Such an improvement will enable us to install longer undulators with planar or helical magnet configurations and minipole undulators with a narrower gap at the short straight sections. By adding 5 straight sections on the 6.5 GeV ring, the Photon Factory will have a total of 18 straight sections for insertion devices. An in-vacuum short period undulator beamline for structural biology is now being constructed and will be commissioned in the fall of 2005. Another in-vacuum undulator X-ray beamline for materials science will be constructed and commissioned in 2006.

Tadashi Matsushita

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Neutron facilities

Japan started atomic energy related activities well behind Western countries after World War II. In the mid 1950s the first nuclear research reactor JRR-1 (Japan Research Reactor No.1, 50kW, now preserved in a museum in Tokai) built by the Japan Atomic Energy Research Institute (JAERI) was used for neutron beam research. Neutron scattering research requiring an MW-class reactor started in the early 1960s when JAERI built the JRR-2, which could produce a thermal power of 10MW, thermal neutron flux or 2×10^{14} neutrons/cm²/sec. There were 9 neutron scattering instruments during its most active period. It was the first neutron source available for inelastic experiments and also played a central role in training

many researchers. It was permanently shut down in 1996, as scheduled, after about 35-years of service. Side-by-side with JRR-2, the JRR-3 (10MW, 1×10^{14} n/cm²/sec, 6 instruments) was built with purely domestic technology for the first time. In the mid 1960s Kyoto University built its 5MW reactor named KUR (3×10^{13} n/cm²/sec, 8 instruments; www-jrri.kyoto-u.ac.jp/) in Kumatori. It is the only MW-class reactor owned by a university. In late 1960s and 1970s, therefore, three medium-size reactors were available for neutron scattering and other beam experiments while several high flux reactors became operational abroad such as the HFBR at Brookhaven National Laboratory (60MW, 8×10^{14} , USA), HFIR at Oak Ridge National Laboratory (85MW, 1×10^{15} , USA), and HFR at the Institut Laue Langevin (58MW, 3×10^{15} , France). Japanese user's strong demand for higher neutron flux by the early 1980s culminated in the refurbishment of the JRR-3 to double its thermal power (20MW, 3×10^{14}) and install a new cold neutron source accompanied with a guide hall building. This refurbished reactor renamed as JRR-3M became fully operational in 1990. Currently it supports 25 neutron scattering, 2 neutron radiography and 2 prompt γ -ray analysis instruments and a total number of about 12,000 users per day (www.issp.u-tokyo.ac.jp/labs/neutron/index.html and www.jaeri.go.jp/).



Fig. 3-3-1 A schematic layout of five major facilities based on an intense proton accelerator for the J-PARC jointly promoted by JAERI and KEK.

Japan is one of pioneers in the field of accelerator-based neutron sources. In the mid 1960s the electron linear accelerator at Tohoku University in Sendai, dedicated to nuclear studies, was tested as an injector to a metal target to produce neutrons. It was then successfully used as a pulse neutron source for neutron diffraction experiments even after a new spallation neutron source was built at KEK (the present High Energy Accelerator Research Organization; <http://kek.jp/>) in Tsukuba in 1980. This neutron source, named KENS, was the first dedicated pulse neutron facility in the world and it has been operated at a proton beam power of 4kW for a total of 17 instruments and a cold source. Several more powerful sources were built abroad such as IPNS at Argonne National Laboratory (6kW, 1981, USA), LANSCE at Los Alamos National Laboratory (80kW, 1985, USA), and ISIS at Rutherford Appleton Laboratory (160kW, 1985, UK). The Japanese community demanded a much stronger pulse neutron source to follow post-KENS. KEK belonging to the Ministry of Education, Science and Culture (MONBUSHO) planned the Hadron Project consisting of four major facilities based on an intense proton accelerator (0.6MW) to be used for neutron scattering, muon science, nuclear and high energy physics. JAERI belonging to the Science and Technology Agency (STA) also planned a MWclass proton accelerator that would provide intense proton beams to two facilities for neutron scattering and R&D for nuclear transmutation. Both were very big projects costing nearly one billion US dollar each. When MONBUSHO and STA merged, it was recommended that both projects merge and be promoted jointly by JAERI and KEK. In 2001 the Japanese Government funded it for the following 6 years (later extended to a 7-year project in 2003). Fig. 3-3-1 displays a layout of the facility, now called J-PARC (Japan Proton Accelerator Research Complex; <http://j-parc.jp/>), which consists of 5 major facilities based on an intense proton accelerator (1MW). According to the plan, proton beams are accelerated by Linac up to 400MeV and transported into the 3GeV rapid cycling synchrotron (3GeV PS in figure) further accelerating up to 3GeV. Most of the beams are transported to the Materials and Life Science Facility (3GeV PS Experimental Area) where both neutrons and muons are produced. This neutron beam facility, tentatively called JSNS (Japan Spallation Neutron Source, 1MW), will have a total of 23 beam lines at which instruments will be installed. A small portion of the proton beams from the 3GeV PS is fed into the 50GeV synchrotron (50GeV PS) for nuclear physics and for long base-line neutrino experiments to be combined with the Super KAMIOKANDE. In the near future, a superconducting Linac will be installed at the end of the 400MeV Linac to further accelerate proton beams up to 600MeV for R&D study of nuclear transmutation.



Fig. 3-3-2 An aerial photograph of the construction site of J-PARC in Tokai Research Establishment of JAERI directly facing the Pacific Ocean. JRR-3M reactor currently operational and JSNS under construction are located within 1km. Photo taken from the right hand side (south) of Fig. 3-3-1.

Fig. 3-3-2 is an aerial photograph of the construction site of the J-PARC taken in February 2004, the fourth year of the 7-year project. One can see both the JRR-3M 20MW reactor-based steady source and the JSNS 1MW accelerator-based pulse source located within 800m of each other on the same campus facing the Pacific Ocean. This co-location of both neutron sources will be a great advantage for neutron science and technology and they will be available to users worldwide. The first neutron beams from JSNS are scheduled in November 2007 and a users program will start in April 2008.

The Japanese neutron community has been dominated by solid state physicists at the forefront of solid state physics and material science particularly in the field of low-dimensional magnetic and strongly-correlated electron systems including high- T_c superconductors and CMR materials. After cold neutrons became available from JRR- 3M in 1990, however, soft-matter scientists and biologists started using the domestic neutron facilities and now account for as many as one quarter of the total proposals. Another innovation in neutron crystallography is a neutron-sensitive imaging plate (IP) specially developed by the JAERI group with Fuji Film Co., which has opened up a new era of structural biology. Another important instrumental development is the wide variety of neutron optical devices such as the magnetic lens, compound prism, and supermirrors cooperatively developed by RIKEN, JAERI and KUR Groups (<http://nnp.riken.go.jp/indexJ.html>). These devices combined with a new neutron source will lead to new instruments to reach an unexplored region of momentum-energy-spin space for promoting new fields of crystallography.

Yasuhiko Fujii, JAERI

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Recent developments in biological crystallography

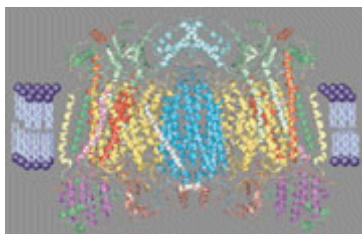


Fig.2-2-1. The structure of bovine cytochrome oxidase

In 1913, one year after Laue's discovery, Nishikawa and Ono of the University of Tokyo successfully observed diffraction patterns from plant and animal fibers. Forty-six years later, M. Kakudo of IPR, founded a laboratory for protein crystallography at Osaka University. This group started to crystallize cytochrome c in 1962. After developing automatic four circle diffractometers and computing programs, they determined the structure of bonito ferrocytochrome c at 2.3 Å resolution in 1973. With the support

of the Crystallographic Society of Japan, M. Kakudo and N. Yasuoka established the Research Center for Crystallography at IPR in 1978 to promote protein crystallography in Japan. In the 1970s, two additional groups were active in protein crystallography. N. Sakabe (Nagoya University) and Y. Mitsui (University of Tokyo) were working on insulin and subtilisin inhibitor protein, respectively. Another protein structure determined during the 1970s was a bacterial protease inhibitor (1977), whose structure was solved by Mitsui's group. Many protein crystallographers were trained in these three groups. In the early 1980s two notable structures, [2Fe-2S] ferredoxin at 2.8 Å (1980) and RNase ST at 2.5 Å (1982), were reported by Kakudo's group and by Mitsui's group, respectively. The structures of Taka-amylase A at 3.0 Å (1980), rice ferricytochrome c at 2.0 Å (1983), cytochrome c3 at 1.8 Å (1984), a complex of subtilisin and its inhibitor protein at 2.6 Å (1984), Bowman-Birk type protease inhibitor at 3.0 Å (1986), [4Fe-4S] ferredoxin at 2.3 Å (1988), aspartate aminotransferase at 2.8 Å (1988), and omega-amino acid: pyruvate aminotransferase at 2.0 Å (1989) were determined during the 1980s.

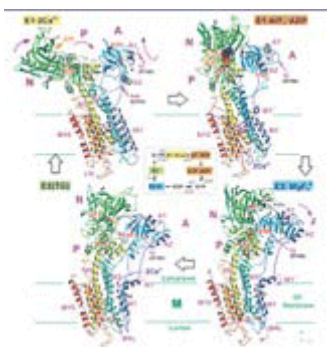


Fig. 2-2-2. The structure of sarcoplasmic reticulum calcium pump.

In the 1990s, new research groups studying protein crystallography were organized by a younger generation of scientists both inside and outside of universities. The number of protein structures determined at high resolution has gradually increased. Eight membrane protein structures have been determined at high resolution using X-ray methods in Japan. In 1995, following an almost 20 year collaboration, T. Tsukihara's group at Osaka University and S. Yoshikawa's group at Himeji Institute of Technology succeeded in the structure determination of a bovine respiratory membrane protein complex, cytochrome c oxidase, consisting of two copies of 13 different subunits (Fig. 2-2-1). This structure, the first membrane protein structure determined from mammalian cells, was a marked breakthrough not only in crystallographic studies of membrane proteins, but also in the field of bioenergetics. Upon examination of the structures of the enzyme complex in different reaction states, these groups proposed a new theory of the proton pumping mechanism (1998, 2003). C. Toyoshima (University of Tokyo) determined the structure of the sarcoplasmic reticulum calcium pump in 2000 (Fig. 2-2-2). He successfully demonstrated the mechanism of calcium pumping by serial structural analyses of reaction intermediates (2002, 2004). T. Okada's endeavor to crystallize a G protein-coupled receptor resulted in successful structure determination by a collaboration of SPring-8 group lead by M. Miyano and R. E. Stenkamp's group of University of Washington in 2000. Collaborating with A. Yamaguchi (Osaka University), three young crystallographers, M. Murakami, S. Nakashima and E. Yamashita, determined the structure of the bacterial multidrug efflux transporter AcrB in 2002. The structure of rat monoamine oxidase A (2004) was the first structure of a membrane protein with an isolated single transmembrane helix. The structures of three other membrane proteins, bacteriorhodopsin by Kouyama (Nagoya University, 1999, 2004), a bacterial photoreaction center by K. Miki (Kyoto University, 2001), and photosystem II by N. Kamiya (RIKEN, 2003) have been determined. Y. Fujiyoshi (Kyoto University) has been working on the technique of cryo-electron microscopy since the 1980s. Collaborating with scientists around the world, he has determined the structures of a number of physiologically important membrane proteins and viruses, including influenza A virus (1994), a plant light-harvesting complex (1994), bacteriorhodopsin (1999), nicotinic acetylcholine receptor (1999, 2003), aquaporin 1 (2000), a voltage-sensitive sodium channel (2001), and others.

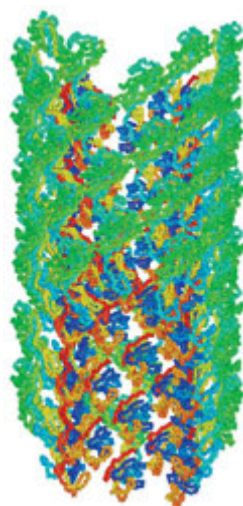


Fig. 2-2-3. The structure of bacterial flagellar.

K. Namba (Osaka University) elucidated the mechanism of bacterial flagellar assembly and function by combining cryo-electron and X-ray structures (1995-2004) (Fig. 2-2-3). A. Nakagawa elucidated the structural organization of a double-shelled RNA virus based on the structure of Rice Dwarf Virus at 3.5 Å resolution (2003). Many other physiologically important protein structures have been determined in Japan since the mid 1990s. Outstanding structural studies on recombination, replication, transcription, and translation have been performed by K. Morikawa (BERI, 1999-2004) and T. Hakoshima (Nara IST, 2000), S. Yokoyama (RIKEN and University of Tokyo, 1995-2004), and I. Tanaka (Hokkaido University, 1997, 1999). After setting up a Structural Biology Center in the Photon Factory, S. Wakatsuki has made significant progress in understanding the structural biology of lysosomal protein transport (2002, 2003).



Fig. 2-2-4. Early version of a Sakabe camera at the Photon Factory

In 2002, the Japanese government started a large structural genomics program, "Protein 3000." In addition to the highthroughput structural genomics approach led by S. Yokoyama (RIKEN), eight target oriented structural genomics projects led by I. Tanaka (Hokkaido University), S. Wakatsuki (Photon Factory), M. Tanokura (University of Tokyo), K. Miki (Kyoto University), A. Nakagawa (Osaka University), and others are included in Protein 3000.

N. Sakabe has been developing IP diffractometers at the Photon Factory since the early 1980s (Fig. 2-2-4). Before SPring-8 began operations, all protein crystallographers were dependent on him for the collection of intensity data. Many Japanese and foreign crystallographers determined a number of novel crystal structures using his detectors at the Photon Factory. The newest version, which has a high quality and high speed detector, was installed at BL-6C in the Photon Factory. S. Wakatsuki has built a new user friendly undulator beamline equipped with a CCD detector. The Photon Factory has one undulator and three bending magnet beamlines and SPring-8 has four undulator and six bending magnet beamlines for protein crystallography. Each beamline has specific features, requiring separate network systems for access. In addition to X-ray beamline facilities, the Japanese Atomic Energy Institute has a neutron beamline facility. A neutron diffractometer dedicated to protein crystals has been developed by Niimura's group (2004).

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FEATURE ARTICLE

Yuji Ohashi



Yuji Ohashi was born in Fukui, Japan in 1941 and studied chemistry at the University of Tokyo. After graduating in 1964 he pursued his interest in crystallography under the supervision of Yoshihiko Saito. He became a research associate at the Tokyo Institute of Technology in 1968 and he received his DSc degree from the University of Tokyo based on the structural studies of reaction intermediates.

In 1977 he found that a chiral alkyl group of a cobaloxime complex was racemized on exposure to visible light with retention of the single crystal form. The inversion process of the chiral group was observed directly from changes in the electron density maps during intermediate stages of the reaction. Such a reaction was called crystalline-state reaction to distinguish it from the usual solid state reactions. Not only small alkyl groups but also bulky groups bonded to the cobalt atom were found to isomerize in the crystalline-state on exposure to visible light. A variety of crystals other than cobaloxime complexes also showed a crystalline-state reaction. Recently a variety of unstable species such as radical pairs, triplet carbenes and triplet nitrenes were analyzed by X-rays, since the photo-produced unstable species were kept in the crystal with retention of the crystalline lattice at low temperatures. Moreover, the photo-excited state of the diplatinum complexes was analyzed by X-rays, irradiating the crystal with UV light at low temperatures.

In order to obtain the intensity data more quickly, a new diffractometer with an imaging-plate detector, R-AXIS RAPID, was developed in collaboration with Rigaku. Moreover, a new photon-counting detector, MSGC, is now being developed in collaboration with Prof. Tanimori of Kyoto Univ. in order to collect an entire dataset within one second.

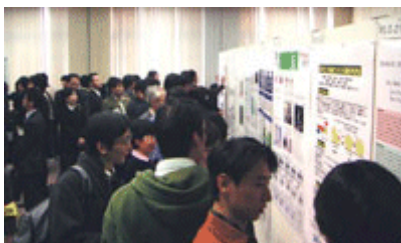
He has been honored by the Crystallographic Society of Japan (1983), the Chemical Society of Japan (2002) and by Harushige Inoue from JST (2002). He has served the scientific community as the Chair of Organic Crystal Committee of the Chemical Society of Japan (2001-2002), Chair of the Japanese National Committee for Crystallography (1994-1997), President of the Crystallographic Society of Japan (1998-1999), President of the Asian Crystallographic Association (1999-2002) and as a member of the IUCr Executive Committee (2002-2005).

MEETING REPORT

2004 annual meeting

Osaka, Japan, November, 2004

The Annual Meeting and General Assembly of the Crystallographic Society of Japan was held at Osaka U., Osaka, Japan, November 16-17, 2004.



Poster session at the CrSJ 2004 Annual Meeting

The meeting featured 3 special symposia, 74 oral and 174 poster presentations covering all aspects of crystallography, and an industrial exhibition. 547 crystallographers attended the meeting, which was the largest number of attendees to date.



(left to right) J. Harada, Y. Marumo, N. Yamada, K. Ohsumi (President), T. Chatake and K. Kusaka.

The three symposia were on “Crystallography of Photo-Induced Phenomena”, “Global environmental problems and Crystallography” and “Forefront of membrane proteins and biological supramolecular complexes studies”.



Noboru Yamada: the Nishikawa memorial lecture.

The lectures “Recent Advances in Photo-Induced Phenomena and Their Time-Resolved Structure Analyses” (H. Uekusa, Tokyo Inst. of Tech), “Single Crystal Structure Analyses of Photo Induced Excited States and Reaction Intermediates using the Low-Temperature Vacuum X-ray Camera on SPring-8 BL02B1” (K. Toriumi, U. of Hyogo), “Photo-induced structural transition probed by steady-state and time-resolved X-ray diffraction” (S. Adachi, KEK-PF), “Photoexcited Structure on Charge Density Level using Powder Diffraction” (K. Kato, JASRI/SPring-8) were included in the first symposium.



Y. Sasada

“Atmospheric Oxygen Evolution Revealed by Crystallography - Reconstruction of Paleoweathering” (T. Murakami, U. of Tokyo), “Crystallography in Environmental Earth Sciences; atmosphere, water, soils, and bacteria” (K. Tazaki, Kanazawa U.), “Regulation mechanism of the crystal orientation in calcium carbonate as biominerals” (T. Kogure, U. of Tokyo), “Surface Environment of the Earth and EM-Mineralogy/Crystallography of nano- to micro-meter scale Fe-minerals” (J. Akai, Niigata U.) were included in the second symposium.

And “The new stage of structure-functional research of membrane - a protein complex - cytochrome c oxidase” (H. Aoyama, RIKEN), “Crystal structure of the complex between Vitamin B12 receptor and Colicin E3” (G. Kurisu, U. of Tokyo), “Crystallization and structural-functional analysis of a bacterial multi-drug efflux transporter” (S. Murakami, Osaka U.), and “Crystal structure and function of the MexAB-OprM antibiotic efflux pump subunits of *Pseudomonas aeruginosa*” (T. Nakae, Tokai U.) were included in the third one. The Nishikawa memorial lecture titled “Development and structure analysis of phase-change optical disk materials” was presented by N. Yamada (Matsushita Electric Industrial Co., Ltd.).

At the Awards Ceremony, the Young Crystallographer Awards went to K. Kusaka (JAERI) and T. Chatake, (Chiba Inst. of Science). At the general meeting, J. Harada (Prof. Emer. Nagoya U.), F. Marumo (Prof. Emer. Tokyo Inst. Tech.) and Y. Sasada (Prof. Emer. Tokyo Inst. Tech.) became Honorary Members of our society.

The local Chair was Y. Kai (Osaka U.) and the Program Chair was A. Nakagawa (Osaka U.). Details of the meeting program can be viewed at wwwsoc.nii.ac.jp/crsj/index-e.html.

Kenji Tsuda

MEETING REPORT

2005 annual meeting of JSSRR

Tosu-city, Japan, January, 2005



Great discussions at the poster session

The 18th Annual Meeting and General Assembly of the Japanese Society for Synchrotron Radiation Research(JSSRR) was held with the symposium of synchrotron radiation facility user's society groups at Sun-Messe Tosu Conference Hall in Tosu-city, Japan, January 7-9, 2005. It was attended by 607 people and included 6 symposia, 96 oral presentations and 356 poster presentations covering all aspects of synchrotron radiation research and technology and 49 industrial exhibits.



Open public lecture "What is the Saga light Source?"

Symposia included "Recent progress on soft X-ray optical elements" and "Now and the future on SR-XRF analysis for biological and environmental sciences", "Recent developments on THz Coherent Scattering Radiation", "Super high-resolution protein structure analysis", "Front-lines of Bio-Nano-microspectroscopy by UV-SX high brilliance SR" and "The role of Synchrotron Radiation in the future: pathbreaking SR utilization for research on excited states". The lectures "The XRF analysis in nano-technology " (H. Ishida, Toray Research Center), " Advanced scientific research in a developing country. – Synchrotron Radiation facility construction in Thailand" (T. Ishii, Suranaree U. of Technology) were presented as keynote lecture.

At Tosu City in Kyusyu island Japan, a new synchrotron radiation facility is now coming out, the Saga Light Source. So, as a special event, the JSSRR lecture, "What is the Saga light Source?" included three lectures, "The Saga Light Source is the reborn Saga refining plant in 21st century" (Y. Furukawa, Governor of Saga prefecture), "What is the synchrotron radiation?"(Y. Kitamura, RIKEN) and "What you can see by synchrotron radiation? (I. Nakai, Tokyo Science Univ.). More than 300 people, including high school students, enjoyed the lectures and asked many questions.



Award-winners of the JSSRR Young Scientist Awards. (from left) O.Shimomura(President of JSSRR), K.Amemiya(Tokyo Univ.), Y.Harada(RIKEN) and W.Yashiro(NIMS).

At the annual Awards Ceremony, the JSSRR Young Scientist Awards were given to K. Amemiya (Tokyo U.), Y. Harada (RIKEN) and W. Yashiro (NIMS). The Local Chair was T. Okajima (Saga Light Source) and the Program Chair T. Kamada (Saga Univ.).

Hiroshi Sawa(KEK), Secretary in public relation, JSSRR

MEETING REPORT

Crystal growth under Popocatepetl

Puebla de los Angeles, Mexico, March, 2005



The Commission on Crystal Growth and Characterisation of Materials of IUCr closed the activity of the triennium 2002-05 on a high note with an international school in Puebla de los Angeles, Mexico, March 7-11, 2005. The International School on Crystal Growth: Fundamentals, Methods and Applications Biological and Nano-crystals was co-chaired by Maria Eugenia Mendoza (Inst. of Physics, U. Puebla) and Abel Moreno (Inst. of Chemistry, UNAM) and sponsored by the IUCr, Sociedad Mexicana de Cristalografia, U. Autonoma de Puebla, U. Autonoma de Mexico, Bruker, Spectramex, Zeiss and Presidencia Municipal de la Ciudad de Puebla.



A group of participants on the staircase of the old university building.

The school was aimed at young researchers, PhD and Master students working in the area of materials science and biological crystallisation. The main objective was to provide the basic concepts of crystal growth along with an overview of growth technologies. The program included a series of tutorial lectures on computer modelling of growth processes, epitaxy of semiconductors, bulk growth of oxides and semiconductors, organic materials for NLO, ferroelectric materials, solution growth of biocrystals, structural studies and defects in real crystals. Though the program was extremely broad, both lecturers and participants recognized that it was useful in order to overcome the strict borders of each one's field of activity and stimulate discussions.



Students and lectures enjoying a typical mexican lunch.

The school was attended by 45 participants, most from Mexico, but with participation from other latin-american countries. The truly international character and cordial interaction between participants and lecturers provided a stimulating atmosphere for scientific as well as general discussions. Poster presentations, organized during one-hour breaks in the morning and afternoon stimulated new contacts and strengthened relations among participants.



Abel Moreno and Maria Eugenia Mendoza, co-chair of the International School on Crystal Growth, holding the school's ensign.

The school was superbly organized, lectures and students were accommodated in two beautiful hotels in the historical centre of Puebla, a colonial city some 120 kilometers from Mexico city, rich in magnificent buildings, museums, baroque churches, lively streets and cultural sites. The lectures were held in the central building of the 400 year old University. The 16 lecturers from Canada, France, Germany, Uruguay, Mexico, Spain, Switzerland, and the USA had the nice surprise of being awarded with a "Reconocimiento" (Acknowledgment) by the Mayor of Puebla for having contributed to the development of the scientific culture in Mexico. The list of lectures and other information is available at www.ifuap.buap.mx/ISCG05/school.html

R. Fornari, Chair

IUCR Commission on Crystal Growth and Characterisation of Materials

MEETING REPORT

MaThCryst 2005

Nancy, France, June 2005

The MaThCryst International Workgroup (www.lcm3b.uhp-nancy.fr/mathcryst/) organized an International School on Mathematical and Theoretical Crystallography at the Faculty of Sciences, U. Henri Poincaré of Nancy, France, June 20-24, 2005. The school was financially supported by the IUCr, ECA, U. Henri Poincaré, French CNRS, Communauté Urbaine Grand Nancy, and Bruker-AXS, and received the formal support of the IUCr commission on Inorganic and Mineral Structures, the Special Interest Group No. 5, "Mineralogical Crystallography" of the ECA, the French Crystallographic Assn, and the LCM3B Nancy crystallography laboratory.

The School was attended by 61 registered participants from 20 countries with different backgrounds (chemistry, physics, mineralogy, mathematics, biology...). Twenty-two young scientists from 13 countries were financially supported, for a total of 8,000 € in grants, including a special grant for French young scientists provided by the French Crystallographic Assn. This heterogeneous public was introduced to several aspects of modern theoretical crystallography by nine invited lecturers: T. Hahn, H. Wondratschek, U. Müller (Germany), M.I. Aroyo (Spain), V. Kopský (Czech Republic), M. Catti (Italy), A. Oganov, H. Flack (Switzerland) and T. Yamanaka (Japan). The School included a poster session, with 23 posters presented: the electronic version of the abstracts is available from the school website (www.lcm3b.uhp-nancy.fr/mathcryst/nancy2005.htm). A special issue of *Acta Cryst. A* will be published with articles from the lecturers and manuscripts submitted by the participants. MaThCryst will organize a Satellite Conference of the ECM-23, XXIII European Crystallographic Meeting in U. Leuven, Belgium, August 4-6, 2006 (details available at www.lcm3b.uhp-nancy.fr/mathcryst/leuven2006.htm).

Massimo Nespolo, organizer of the MaThCryst School
massimo.nespolo@lcm3b.uhp-nancy.fr

MEETING REPORT

Recent advances in X-ray powder diffraction

Assiut, Egypt, November 2004



This is the 9th Workshop and School organized by the Egyptian Society of Crystallography and Application (ESCA) and the National Committee of Crystallography. The workshop is the 9th in number but is the 2nd in Powder Diffraction. The first Powder Diffraction Workshop about Rietveld methods was held in Cairo in the National Research Center in 1990. Among the lecturers was Prof. Rietveld himself and Prof. Young the developer of the method at that time. The workshop was sponsored by the Academy of Scientific Research and Technology, Assiut U, and the IUCr.



About 63 participants attended; most from universities and institutions in Egypt and the others from eight different countries (five from Arab Countries, one from India and two from Europe). The program focused on the recent advances in *ab-initio* structure and microstructures analysis using different programs. The lectures were given by highly specialized eminent lecturers (C. Giacovazzo, A. Le Bail, R. Von Dreele, J. Schneider, R. Shirley and A. W-Aladine). 14 posters were presented. The IUCr grant and the money which was specified for the organization were given to seven post graduate students as follow: one from India, two from Europe, one from Yemen, one from Syria and two from Morocco. Fifteen other grants were given to M.sc Egyptian students

Two main social activities took place; a three hour boat ride on the river Nile where everyone enjoyed the good weather, the green lands cultivated with crops and palm trees on one side of the river and different styles of buildings on the other side. Another trip was arranged to see the Virgin Mary Cave with its beautiful church inside and a convent on top. The Cave is of special interest because it was used by the Virgin Mary and Child to hide from the Romans. Another walking trip was made to the University's Olympic City.

The closing ceremony was started by the president of Assiut U.. He thanked the lecturers for the good work they did and for being guests of the Assiut U. and he wished for them and the participants an enjoyable stay in Egypt. He ended his talk by presenting the University Arm (Shield) to each lecturer. Farid Ramadan Ahmed Poster prize was given to the best poster among the Egyptians. The ESCA Poster Prize was given to two Europeans. The closing Ceremony ended with a round table discussion concerning topics for future meetings.

Karimat El Sayed

AWARDS AND PRIZES

Bricogne receives honorary doctorate



Gérard Bricogne bows to the dignitaries and audience after having received his honorary doctorate from Uppsala University

On January 28, 2005, Gérard Bricogne (Global Phasing Ltd, Cambridge, UK) received an honorary doctorate from Uppsala U. in Sweden in recognition of his development of fundamental crystallographic methodologies that have revolutionised the structure determination of biological macromolecules. Bricogne has been Directeur de Recherche at LURE (Orsay, France), and has held a Howard Hughes International Research Scholarship while at LMB Cambridge. He is the recipient of numerous awards, notably the Prix Grammaticakis-Neumann of the French Academy of Sciences, the Dorothy Hodgkin Prize of the British Crystallographic Assn, and the Patterson Award of the American Crystallographic Assn. He is a member of the French Academy of Sciences (Section for Mathematics) and held the 1992/93 Tage Erlander Guest Professorship of the Swedish Research Council.

He has worked on developing methods that enabled the use of non-crystallographic symmetry for protein and virus structure determination. He also worked on the theoretical underpinnings for the application of maximum likelihood methods to macromolecular crystallography.

He has founded a not-for-profit company (Global Phasing Ltd.) that is essentially devoted to carrying out his research and development work as if it were in academia. The Cambridge-based company develops innovative methods and software for the determination and refinement of macromolecular crystal structures and is supported by a consortium of pharmaceutical and drug discovery companies, and by participation in EU-funded research networks. All of the software is made freely available to academic crystallographers.

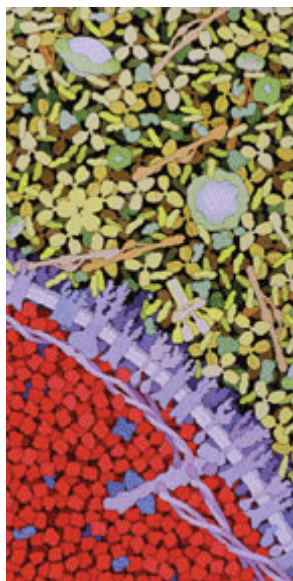
On the occasion of his visit to Uppsala in January, Dr. Bricogne (and his colleague C. Vornrhein) presented a much appreciated hands-on workshop on the use of his latest methodologies.

Previous macromolecular crystallographers who have received an honorary doctorate from Uppsala U. include Wayne Hendrickson, Michael Rossmann and Eleanor Dodson.

Gerard Kleywegt and Alwyn Jones (Uppsala U.)

AWARDS AND PRIZES

2005 Art in crystallography winners



First Place by David S. Goodsell.

In May, 2005, the winners of the first ACA Art in Crystallography competition, sponsored by the ACA Newsletter together with the ACA Council, were announced. First place went to David S. Goodsell for *Blood 2,000,000X*; second place to Edgar Meyer for *Cortisol*, and Honorable Mention to Dan Anderson for *Be Fruitful and Symmetrize*. The entries were posted on the web prior to judging.

An article on prize winners appeared in the Summer, 2005 ACA Newsletter, which featured the winning entry on the cover. (An art entry was also on the cover of the Winter, 2004 issue.) Prints of all the 2005 entries were displayed at the Orlando ACA meeting and were sold in a silent auction during the meeting, with proceeds donated to the Student Travel Fund. Entries to the 2006 Art in Crystallography competition, open to all ACA members, are welcome at any time. Entries are accepted in the form of images emailed to either of the ACA Newsletter Editors (conniechidester@earthlink.net or flippen@rcsb.rutgers.edu). Each entry should be accompanied by a paragraph explaining the science and the method of producing the image. A photo of the artist will be appreciated, but is not required.

Connie Chidester

AWARDS AND PRIZES

Academy membership for Alexander Wlodawer

Alexander Wlodawer, who was born in Poland and maintains very active collaborative links with Polish science, has been elected a foreign member of the Polish Academy of Sciences (PAN). PAN has 350 national members (full and corresponding) and about 200 foreign members. Alex was elected by the vote of the General Assembly of the Academy, after a very competitive nomination by the Division of Biological Sciences. The membership was awarded by Andrzej Legocki, President of the Academy, on June 25, 2005, during the opening ceremony of the Inhibitors of Protein Kinases conference held in Warsaw. This honorable distinction recognizes his contribution to the advancement of structural biology, including discoveries fundamental for the development of drugs against AIDS and cancer and for our understanding of enzyme action. His accomplishments are linked to his research at the National Cancer Inst.- Frederick (USA), where he heads the Macromolecular Crystallography Laboratory.

Mariusz Jaskolski, Poznan, Poland

AWARDS AND PRIZES

Jones receives Patterson Award



Louis Delbaere, ACA President presents T. Alwyn Jones with the Patterson Award

This year, the ACA bestowed its coveted A. Lindo Patterson Award on T. Alwyn Jones, FRS (Uppsala U.), in recognition of his pioneering work in the development of computer-graphics software for macromolecular model building. Jones obtained his PhD in biophysics from Kings College in the early 1970s, and then moved to Munich, where he began the development of the famous FRODO program (initially called INTER). After moving to Uppsala (Sweden) in 1979, he continued the program's development, but later began work on a successor that he redesigned from scratch. This successor is called "O" for reasons Jones steadfastly refuses to divulge. For more than two decades the vast majority of all macromolecular crystal structures were built with these two programs, a fact recognized by the ACA award, as it had been previously by the Royal Swedish Academy of Sciences through its Aminoff Prize (shared with Axel T. Brunger in 2003). Ever since using Ramachandran plots to select high-quality protein crystal structures for inclusion in O's database in the mid-1980s, Alwyn has also had a keen interest in model validation, and his Nature commentary (with C.-I. Brändén; Nature 343, 687-689 (1990)) today stands as a landmark publication in this important area of macromolecular crystallography.

A special symposium on "Macromolecular Model Building and Validation" was organized as part of the meeting in Orlando, FL. Jones gave a very entertaining historical overview of his work in the areas of model building and validation. This was followed by contributions from people involved in model building or validation. P. Emsley (York U.) talked about his program COOT; G. Kleywegt (Uppsala U.) discussed a project that was initiated by Jones, namely the Uppsala Electron-Density Server (EDS: <http://eds.bmc.uu.se/>); T. Terwilliger (Los Alamos) described automated iterative model building and density modification in the context of the Phenix software project; and J. Richardson (Duke U.) discussed the validation software being developed at Duke U. to provide tools that can not only diagnose problems (validation), but also propose methods for fixing them (<http://kinemage.biochem.duke.edu/molprobity/>).

Excerpted from Gerard Kleywegt's report for the ACA Newsletter

AWARDS AND PRIZES

ACA announces 2006 Buerger and Warren Award winners

To be presented at the ACA meeting in Honolulu, HI, July 22-27, 2006:

Martin Buerger Award



Helen Berman (Rutgers, The State U. of New Jersey). The Buerger Award recognizes a mature scientist who has made a contribution of exceptional distinction in an area of interest to the ACA. The award recognizes Helen's lifetime work in the pioneering development of information services for the global community of researchers who both produce and use macromolecular structural data. A session on systematic approaches to structural biology is planned.

Bertram E. Warren Award



Charles F. Majkrzak (National Inst. of Standards and Technology). The Warren Award recognizes an important recent contribution to the physics of solids or liquids using X-ray, neutron, or electron diffraction techniques. Charles is being cited for his seminal contributions to the development of neutron reflectivity and for his pioneering work in the exploration of many issues in interface science using this technique. A session on materials is planned.

NOTICE

Announcements

Congratulations to the winners of the IUCr journals poster prizes!

The prize for the best crystallization poster from a young scientist at the 17th West Coast Protein Crystallography Workshop (Pacific Grove, CA, USA; March 20-23, 2005) was awarded to Serdar Uysal and team (U. of Chicago, IL, USA and Genentech, Inc., San Francisco, CA, USA) for the presentation “Crystallization Chaperones”. The selection committee consisted of H. Einspahr, P. Fitzgerald and A. McPherson, all members of the editorial board of the IUCr’s latest journal, *Acta Crystallographica Section F: Structural Biology and Crystallization Communications* (journals.iucr.org/f). The winner was presented with a copy of *International Tables for Crystallography Volume F, Crystallography of biological macromolecules*.

The winner of the equivalent competition with the same prize at Recent Advances in Macromolecular Crystallization (Le Bischenberg, France, May 8-11, 2005) was Claude Sauter (Richard Giegé laboratory, IBMC-CNRS, U. of Strasbourg, France) for his poster “Crystallization in Gels: Principles and Practical Tips”, judged by C. Betzel (U. of Hamburg, Germany), H. Einspahr and A. McPherson.

Is your entry in the World Directory of Crystallographers up to date?

The new version of the IUCr’s free online directory of crystallographers and other scientists employing crystallographic methods allows you to modify your own entry via the web at any time and includes provision for multiple addresses, URLs, photographs, audio clips and more scientific and general interests. To update or add your entry, please visit <http://wdc.iucr.org>. Please note: readers who were in the 10th edition of the directory but have not yet checked their entry are urged to log in at the above address using their IUCr ID and password. Please direct any queries to wdc@iucr.org.

OBITUARY

Lyudmila Gorogotskaya (1935-2005)



Lyudmila Gorogotskaya, well-known investigator of mineral structures, died of cancer on January 4, 2005, one month before her seventieth birthday.

Lyudmila Gorogotskaya graduated from the crystallography professorship course of the Moscow University where she was a follower of Prof. G.B. Bokii. In 1967 she took the Doctor's degree for her thesis 'Crystal structures of singenite and chukhrovite, their niche in structural classification of sulfates'.

For most of her life she worked at the Kiev Institute of Geochemistry and Physics of Minerals of the Ukrainian Academy of Sciences, at the experimental mineralogy department. She was engaged in synthesis of minerals and their analogues and studies of their crystal structures. She determined the crystal structures of new minerals, such as X-andalusite and ceisestibantite, and studied novel layer silica modification by powder diffraction to prove their structural individuality and develop structure models.

She published over 80 papers on crystallography and structural mineralogy in leading scientific publications of the USSR, Russia, and Ukraine.

Lyudmila was keen on gymnastics and took a great interest in philosophic systems of physical and moral improvement. She had a happy family and a lot of friends.

Her relatives, friends, and colleagues from Moscow, Kiev, Novosibirsk, and Kharkov will always have affectionate memories of Lyudmila Gorogotskaya – Lyusi (for friends and relatives).

N.V. Podberezskaya, A.A. Valter, S.V. Borisov, V.V. Bakakin,

OBITUARY

Mary Rosaleen Truter (1925-2004)



Gordon Cox and Jackie Truter at the 1954 Paris IUCr

“Jackie” Truter (Lady Mary Cox) died from leukemia on 26 November 2004. Her career in X-ray crystallography began in 1945 and at her death she was still active as Visiting Professor in the Chemistry Department at University College, London. She was the widow of Sir Gordon Cox FRS.

Mary Rosaleen Jackman, “Jackie,” attended Imperial College, London, where A.J.E. Welch, who had given excellent lectures on crystal chemistry, started her on research with X-ray powder photography. After hearing Sir Lawrence Bragg at the Royal Institution she “was hooked on crystallography.” After graduation she got a job as Assistant Lecturer in the Dept. of Inorganic and Physical Chemistry at Leeds U. advertised for someone with “an interest in, but no necessary knowledge of, crystallography.” In 1947 she married Eric Truter, whom she had met as a chemistry student at Imperial College, a marriage that lasted until 1965.

She obtained her PhD degree, based on research to determine the crystal structure of nitronium perchlorate, from U. of London as an external student while carrying a heavy teaching load at Leeds. With her research students she achieved a considerable reputation with a series of papers on trimethyl platinum compounds, arising from syntheses by R.C. Menzies dating back to 1928. She was promoted to Reader in Structural Chemistry in 1960.

In 1966 she was appointed Deputy Director of a new Agricultural Research Council (ARC) Unit of Structural Chemistry at University College, London, and was soon made a Professor. The charge for her Unit, considered a risky idea at the time, was to look for complexes of alkali and alkaline earth metal cations in order to understand and even emulate the discrimination shown between sodium and potassium. They were indeed able to make some complexes and subsequently to determine the crystal structures of several of Pedersen’s crown ether complexes. (Pedersen, Nobel laureate 1987, had shown by 1967 that macrocyclic ethers extract metal salts into non-polar solvents and act selectively on these metals. He spent three months in the Unit in 1969.) Many papers were published including her 1973 review in *Structure and Bonding* “Structures of organic complexes with alkali metal ions” which was an ISI Citation Classic in 1989. She received a Chemical Society Award for Structural Chemistry in 1976. In 1977 the Unit was renamed the Molecular Structures Department and moved to new accommodations at the Rothamsted Experimental Station in Hertfordshire. The group had some very productive years, but in 1984 Mrs. Thatcher’s cuts of research that was considered “too basic” could no longer be staved off. The group was dissolved and Jackie moved to University College where she did some teaching and continued her research.

Jackie married Sir Gordon Cox, then Secretary of the ARC, in 1968. Gordon suffered increasing ill-health from 1992, and he died in June 1996. (He had retired from the ARC in 1971.) Jackie’s own leukemia was first diagnosed in 2002. In periods of remission, she continued to visit the College. She died in November 2004.

Especially as a younger woman, Jackie cut an attractive figure, elegantly dressed and independently stylish. She was a founding member of the BCA, a past chairman of the CCG and a trustee of the CCDC.

At Rothamsted colleagues were always impressed with her dedication to the work, to her staff and students and to the laboratory. Her many friends in the UK and around the world mourn her passing.

Durward Cruickshank

taken from the ACA Newsletter, Summer