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Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President



Henk Schenk

Watching the Olympic Winter Games it strikes me that more than 75 countries are participating. Because the games are devoted to the 'freezing' sports, this is only a subset of all of the countries in the world. In the Summer Olympics at Sydney as many as 200 countries participated.

The International Council for Science (ICSU) organizes the field of science and the IUCr is one of its 26 scientific members. ICSU has national members too, but less than 200 because science is not on the agenda everywhere in the world. Still ICSU has 98 members in three categories: Full Members (75), National Scientific Associates (15) and National Scientific Observers (8). Although crystallography is not pursued in all ICSU countries, the number of countries represented in our General Assembly is much smaller than the number with active crystallographers. Rather than the 40 Adhering Bodies of today we should strive for a much larger membership. It might be necessary to relax or replace a few rules or we may need to think about a new category of National Scientific Associates, but it is worth doing.

Activities are already underway towards increasing the number of members. Two new crystallographic societies have been founded and, in our view, membership in the IUCr goes hand in hand with local organization. So these new societies may well lead to new members. Last year the Hellenic Crystallographic Society was founded in Athens and I have heard from Dr. Irene Mavridis that our Greek colleagues wish to join the IUCr in the near future. On February 1, 2002 the Moroccan Crystallographic Society (ACM) was founded by 80 crystallographers. Prof. Abdelmalik Thalal organized the first Moroccan School of Crystallography in Marrakech, attended by 100 participants from Morocco and Europe. It had a very good programme and excellent organization. I found it particularly encouraging to see more than 40 young scientists actively participating in the discussions. The last afternoon of the school was devoted to the birth of the association, and a strong board with Prof. Abdelkader Mokhlisse as President was formed. It is also the intention of our Moroccan colleagues to join the IUCr. I was told that by the end of the year a similar School would be held in Algeria. The IUCr fully supports these initiatives.

This brings me to my last point. Once more I would like to draw your attention to our Journals Grant Fund (JGF). This fund has been established to help institutions in developing and emerging countries to subscribe to our journals. Institutions have to pay a small part of the subscription fee themselves, perhaps as little as 15%, and the rest of the fee is paid through the JGF. Applying institutions should indicate the maximum amount they are able to contribute themselves, so this is a very open system that tries to take the world's economic differences into account.

This week we reviewed an application from Indonesia. However, in my view the number of grants we award grows too slowly. So applications are heartily welcomed. Forms can be found on the *Crystallography Journals Online* website.

Henk Schenk

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EDITORIAL

Editorial



Make plans to attend the 19th IUCr Meeting in Geneva now. Our Geneva meeting update appears on page 30. No other crystallography meeting reflects so fully the broad range of crystallographic research and brings together thousands of Crystallographers from throughout the world. Because the field is still young, this is a golden opportunity for young people to meet many of its pioneers. Because the technique is so powerful and vibrant and the areas of application are so diverse, it gives us all an opportunity to take a fresh look at the opportunities that lie ahead.



Everything you ever wanted to know about KFeF_2 . A poster on lattice dynamics presented at ECM20 by K. Galicka, A. Slodczyk, *et. al.*

In this issue of the *Newsletter*, for the first time, we have a report from a group with a long history, the French Crystallographic Assn and reports from an emerging communities, in Morocco and Turkey. There are still many countries in our union from whom we seldom receive news. If you are in one of these countries, let the rest of the world know what you're doing.

Some photographs from ECM20, Krakow, appear in the pages of this issue. The next issue should include reports and more pictures from the 2001 ECM, AsCA and ACA meetings. We regret that our publication schedule has been running late. We are trying to correct this. The newsletter is placed on the web when it is sent to the printer. You can view it weeks before your hard copy arrives at www.hwi.buffalo.edu/iucr.



The ECM20 conference banquet at the Royal Palace in Niepolomice, Poland.

LETTER TO THE EDITOR

Letter to the editor

Dear Bill

The bionet.crystallography electronic newsgroup is a useful electronic resource for biological crystallography, providing a forum for general discussion, and a place to post notices such as job advertisements or synchrotron beamline availability. However, in the past year this resource has become a disgraceful collection of spam. To rectify the situation, I have agreed to become moderator of the newsgroup, which means that spam is deleted by me rather than posted to the group. This relatively minor (but satisfying!) task will be made more rewarding if the intended audience – the crystallographic community – makes more active use of the newsgroup again. To subscribe (i.e., receive posts by e-mail) or to browse recent messages, see www.bio.net. To post messages, send e-mail to xtal-log@net.bio.net or xtal-log@net.bio.net.

Cathy Lawson

LETTER TO THE EDITOR

Letter to the editor

Dear Bill

I just got my *IUCr Newsletter* Vol 9 No 3 2001. Please can you look at page 11, the report of the Dorothy Hodgkin Landmark.

Please note that this celebration was organized by the UK Royal Society of Chemistry, NOT the UK Royal Society. Further details can be found on the BCA website <http://bca.cryst.bbk.ac.uk/BCA/Cnews/2001/RSC.html> including some images of the presentation and the plaque itself.

Kate Crennell

MISCELLANY

The Structures of Life

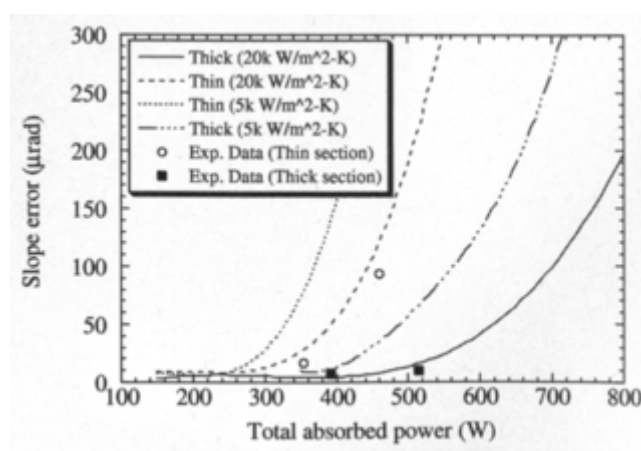
The Structures of Life is a science education booklet, recently published by the National Institute of Health (NIH) geared toward an advanced high school or early college-level audience. It explains how structural biology provides insight in health and disease. It contains a general introduction to proteins, a chapter each on X-ray crystallography, NMR, and structure-based drug design. It, and other science education booklets published by the NIGMS component of NIH are available free of charge. For further information e-mail pub_info@nigms.nih.gov, or order online at www.nigms.nih.gov/new/publist.html.

Nonlinear thermal-distortion predictions of a silicon monochromator using the finite element method

G. Tajiri, W.-K. Lee, P. Fernandez, D. Mills, L. Assoufid & F. Amirouche, *J. Synchrotron Rad.* (2001). 8, 1140-1148

Sometimes Nature provides us with perfect gifts. What would synchrotron radiation be without the perfect silicon crystals that are so valuable as monochromators, polarizers, and analysers in most beamlines? Nature offers the physical basis to grow perfect silicon crystals, engineers in the semiconductor industry have learnt to master the process of producing huge perfect monocrystalline ingots and the makers of synchrotron X-ray optics are capable of transforming the material into optical elements for X-ray beam conditioning. There is a further gift from Nature: at 125 K the thermal expansion of silicon is zero while the thermal conductivity increases threefold with respect to room temperature. This property is extremely valuable because it decreases the thermal deformation generated when cooling silicon crystal optics exposed to undulator or wiggler beams that have heat fluxes comparable to that at the sun's surface. At room temperature the quality of the X-ray beams emerging from modern storage rings would be greatly deteriorated. Nowadays, most high heat load monochromators in beamlines at third-generation storage ring sources are cryocooled. The history of cryogenically cooled silicon monochromators has been described by Bilderback *et al.* (2000).

Because sources tend to become stronger and fourth-generation sources are under discussion, the question arises as to how far we can go with power loading before cryogenic cooling fails. Another important question is how accurately can the thermo-mechanical response and the diffraction properties of the cooled crystals be predicted? The modelling exercise starts with finite element analysis (FEA), in which the piece of material, heated on one side and cooled on the other, is subdivided into many small volumes (the 'mesh'). The computer calculates the temperature distribution and the overall shape of this piece by adding up the contributions of all the small, more or less expanding elements. FEA has been widely tested and gives very reliable results — if correctly applied. The latter *sine qua non* condition has been a challenge for some time. In most of the extensive work done over the past many years it was assumed that the radiation is absorbed at the surface or very close to it. The validity of the assumption depends on the spectral distribution of the incoming beam and on the Bragg angle.



Comparison of thick-section and thin-section thermal distortions.

The work by Tajiri *et al.* has the great merit of having studied the thermal deformation taking into account the depth distribution of the absorbed power. A very detailed FEA was applied to a directly cooled crystal developed at the Advanced Photon Source (Argonne, IL, USA). It was clearly shown that

the penetration depth effect must be considered. The crystal investigated had a thin and a thick section. The thin section was prepared because it was believed that less power absorption would lead to less thermal deformation. Both the calculations and the experimental data for silicon 111 and 8 keV showed that the opposite was true. This can be explained by the strong nonlinearity of the cryogenic cooling process. The cooling of the thin section was much less efficient than in the thick section so that the thin part of the crystal heated up far above the ideal temperature of 125 K and thus thermal deformation was much greater. For the thick section the thermal slope error (see figure), i.e., the deviation from flatness averaged across the beam footprint, stayed below about 10 μrad up to a total absorbed power of 500 W in a beam cross-section of $2 \times 3 \text{ mm}^2$. For higher heat load, the slope error suddenly increased — a runaway effect that can create strong instabilities. It also reveals that a heat exchange coefficient measuring the efficiency of the heat transfer from liquid nitrogen to silicon of $20 \text{ kW m}^{-2} \text{ K}^{-1}$ was appropriate. Although more experimental data are needed for full confirmation, questions about the limits and the accuracy of the predictions mentioned above may soon be answered.

If future machines such as the 'ultimate storage ring' (Ropert, 2001) generate still higher X-ray power, at least three avenues to solve the problem can be envisaged: spreading the beam on the surface of the cryocooled silicon crystal by asymmetric and inclined diffraction geometries, using isotopically pure silicon that has much enhanced thermal conductivity at even lower temperatures, or using single-crystal diamonds that have ultimate thermal performance and are already in use on several beamlines. All these developments will require further studies of the kind described by Tajiri and co-workers.

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Ropert, A. (2001). *Proc. SPIE*, **4501**, 3–16.

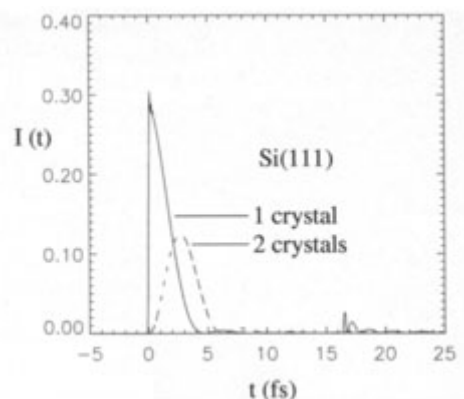
Reviewed by Andreas K. Freund

European Synchrotron Radiation Facility, Grenoble, France

Dynamical diffraction of ultrashort X-ray free-electron laser pulses

S.D. Shastri, P. Zambianchi & D.M. Mills, J. Synchrotron Rad. (2001). 8, 1131-1135

Nature can be tough with humans. It tells us that there are limits. For example, if we want to measure the energy of a particle (or a wave) very accurately we cannot do this in an 'ultrashort' time. Conversely, if we use a very short radiation pulse of length Δt to determine its energy there will be a 'natural' error bar ΔE given by the well-known uncertainty relation $\Delta E \Delta t \geq 2.35^2 h/4\pi$ where h is Planck's constant. (The factor 2.35^2 takes care of the fact that we consider the full width at half maximum of Gaussian distribution functions.) This is precisely what the paper is about: it describes how a crystal would respond to a hypothetical pulse of infinitely short duration. Because the crystal is perfect, the diffraction process is starting from results of dynamical theory obtained for the angular or energy response of a perfect crystal in the steady-state plane-wave approximation. The Darwin-Prins curve is the input for the subsequent calculations of kinematical type using a 'continuous superposition' of Green's functions. The result is, as can be expected, a temporal smearing of the incident delta function. Numerical results were calculated for the 111 and 444 reflections from silicon in the symmetrical Bragg case. Does this semidynamical approach give physically reasonable results?



Delta-function-induced transient reflected intensity at 8 keV from one and two Si(111) Bragg crystals of thickness 10 μm .

There is another way of looking at the problem. For a given X-ray wavelength the beam has to penetrate a certain depth into the crystal to be fully reflected and to achieve the nominal monochromaticity of the reflection used. Although this penetration or extinction depth t_{ext} (I_0/e -depth perpendicular to the netplanes, I_0 is the incident intensity) varies as the crystal is swept across the Bragg angle, its average value can be formally related to the relative spectral resolution $\Delta E/E = d/t_{\text{ext}} = 1/N$ where d is the spacing between the lattice planes and N the number of planes contributing to the reflection. The time delay Δt times c (the speed of light) per lattice plane is just the X-ray wavelength (Bragg's law). Then the total delay between the part of the incoming intensity reflected from the surface and the one coming from an extinction depth below the surface is N times the wavelength. From this we get $\Delta E \Delta t = h$, which agrees to within a factor of 2.5 with the relation given earlier. Inserting numbers: for 8 keV and the silicon 111 reflection ($\Delta E/E = 1.35 \times 10^{-4}$) we get a time delay of 2.8 femtoseconds (fs) for the $I_0/2$ depth. This agrees pretty well with the value of 2.0 fs from the impulse response calculations shown in the figure. Therefore, the two results from dynamical theory interpreted in a kinematical fashion are consistent and appear to be physically reasonable. It is important to note that a full dynamical approach of time-dependent diffraction by perfect crystals starting with the basic equations from Zachariasen (1945) gave a very similar result: 1.6 fs for 12.4 keV corresponding to 2.5 fs for 8 keV radiation

(Sheppard *et al.*, 2001). The result for a double nondispersive reflection is also shown in the figure and one can distinguish an echo coming from the back of the 10 μm thick crystal too. The shape is easy to understand: the intensity gradually decreases as the beam penetrates into the crystal and hence the part of the radiation coming later is less intense.

The theory was then applied to the output of a free-electron laser (FEL), a presently proposed fourth-generation source where a strongly bunched and highly intense electron beam is sent through a long undulator placed after a linear electron accelerator. Under certain challenging conditions self-amplified spontaneous emission takes place starting from noise. In this way the X-ray laser spouts out about 200 fs long bunch trains of many very short ($\geq \text{fs}$), Fourier-transform-limited and extremely intense spikes with strongly fluctuating intensities. The radiation is laterally coherent. The second part of the paper describes what will happen to this hedgehog-like pattern when it is sent through a monochromator. As can be expected, the individual spikes are more or less washed out, according to the degree of monochromaticity achieved. Because the Fourier transform of the time spectrum is a spiky energy distribution, the intensity after transmission through a crystal monochromator shows strong fluctuations, 12% (r.m.s.) for silicon 111 and as much as 56% (r.m.s.) for silicon 444. The time and spectral distributions will vary because each bunch train is different.

All these results are of high interest for time-resolved X-ray diffraction and the future use of FELs. They show that a simple picture of short pulse diffraction can give very realistic results, even on a quantitative level. They also show that we will certainly want to have seeded FELs that would give smooth time and energy distributions. Of course, they confirm that experiments requiring very high energy resolution cannot be carried out on such sources. Finally, an amusing question arises: the diffraction process in the crystal gives priority to monochromaticity, why? It could have chosen to keep the pulse length constant and to smear out the bandpass ... in full agreement with the uncertainty relation.

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Reviewed by Andreas K. Freund

European Synchrotron Radiation Facility, Grenoble, France

MEETING REPORT

2001 annual meeting of CrSJ



Takao Matsuzaki, Fujiko Iwasaki, Yuji Ohashi, Mrs. Soriano Garcia, Michiyoshi Tanaka, Matt Sakata. The Annual Meeting 2001 and General Assembly of the Crystallographic Society of Japan was held in Nagoya, Japan, in October, 2001. This meeting featured 39 oral presentations (6 invited lectures) in three simultaneous sessions and 119 poster presentations covering all aspects of crystallography. Over 270 crystallographers attended to hear and view the presentations and the exhibition of 7 industrial companies.



Reiko Kuroda presented her talk about the crystal structure-color relationship.

Invited lectures included: Crystal and magnetic structure analysis with a 4-circle neutron diffractometer (Y. Noda, Tohoku U.), Humidity-dependent phase transition of nucleosides and nucleotides. (Y. Sugawara, Kitasato U.), A triple mutant of bovine pancreatic phospholipase A₂ (V. Rajakannan, U. of Madras, India), X-Ray Optics for Dark Field Imaging (M. Ando, KEK-PF), Structures and colors of crystals of binaphthol and benzoquinone (R. Kuroda, U. of Tokyo), Human Hematopoietic Prostaglandin D Synthase and Anti-allergic drug design (T. Inoue, Osaka U.).



Poster Session.

At the annual CrSJ Awards Ceremony, the S. Nishikawa Award was presented to N. Sakabe (Foundation for Advancement of Int'l Science), Research Awards were given to K. Miki (Kyoto U.) and Y. Amemiya (U. of Tokyo); and the Young Crystallographer Awards went to G. Kurisu (Osaka U.) and H. Takakura (NIMS, Japan). The banquet was held with special guest, Manuel Soriano Garcia (the first president of Mexico Crystallographers Soc., Circuito Exterior Ciudad U., Mexico).

A full program of the meeting can be viewed at CrSJ home page wwwsoc.nii.ac.jp/crsj/index-e.html. The Local Chair was Makoto Sakata (Nagoya U.) and Takashi Yamane (Nagoya U.) was Program Chair.

MEETING REPORT

Crystallography in Turkey



Participants at the 1st Turkish Crystallographic Assn Meeting, October 2001 in Ankara, Turkey.

In the mid 1960's Ali Fuat Cesur of Ankara U. started an X-ray crystallography laboratory, which remains active today. In 1970 a new laboratory for structural research was established at Hacettepe U. in Ankara, Turkey, under the leadership of Dincer Ulku. Today this laboratory publishes 30-40 structures every year in internationally refereed journals and it is the leading centre of X-ray crystallography in the country. Since 1999 a rotating anode X-ray generator has been in operation in the same department. In 1998 Kırıkkale U. established an X-ray crystallography laboratory, equipped with a full circle fully automated unit and a TEM. Several X-ray powder diffraction units exist scattered across the country.

Targets for crystal structure analysis in Turkey include inclusion compounds such as Hoffmann clathrates, polynuclear coordination complexes of transition metals with unusual magnetic properties, biologically active molecules, intermetallic compounds, molecular modeling and synthetic metallic materials.

The recently formed Turkish Crystallographic Assn presently has 60 registered members, one fourth of whom are senior scientists. The European Crystallographic Assn welcomed the Turkish Crystallographic Assn at its General Assembly in Cracow in August 2001 as a new member. Work is in progress to apply for a membership in the IUCr.

For more information contact dulku@hacettepe.edu.tr or visit www.kristalografi.org

Dincer Ulku

MEETING REPORT

Third national congress in Mexico



The Third Mexican Crystallographic Congress, hosted by the U. of Sonora in Hermosillo City, México, in November 2001, was organized by the Mexican Crystallographic Society (SMCr) and the Mexican Committee for Crystallography. It was attended by 150 people and included eighteen plenary lectures, 117 oral and poster presentations, four courses, three workshops, an exhibit of mineral crystals, and an industrial exhibition.

Plenary lectures included 'From crystals to rocks, a natural bridge between physics and geology' (F. Ortega, UNAM), 'Mineral spectrometry' (M. Ostroumov, Michoacán), 'Structure, properties and simulation of minerals' (L. de Pablo, UNAM), 'Social relevance of Crystallography' (G. Salas, Sonora), 'Biologic macromolecules' (M. Soriano, UNAM), 'Recognition and linking sites in proteins' (A. Rodríguez, UNAM), 'Structure and function of topoisomerases' (A. Mondragón, Illinois), 'The energy landscape of proteins at 0.54 Å resolution' (M. Teeter, Massachusetts), '2- dimensional X-ray microdiffraction' (U. Preckwinkel, Wisconsin), 'Pressure-induced phase transitions' (B. Winkler, Germany), 'High resolution X-ray diffraction of semiconductor materials' (S. Bates, Colorado), 'Intermolecular interactions' (M.J. Rosales, CINVESTAV), 'Identification of expandable clay minerals' (R.W. Berry, California), 'Phase diagrams for mixed oxides in Sol-Gel' (T. López, Mexico), 'Mapping and visualization' (B. Stec, Texas), 'K₃Lu(PO₄)₂: a promising γ-ray scintillator' (J.M. Farmer Tennessee), 'Electron crystallography of human dental enamel' (J. Reyes-Gasga, UNAM), and 'Understanding grain boundary structure' (D. Romeu, UNAM). Courses on 'Crystal growth' (H. Riveros UNAM, J. Olson, Colorado, and A. Moreno, UNAM), 'Macromolecular crystallography' (A. Mondragón, Illinois), 'Diffraction in electron microscopy' (M. Ávalos, California, and A. Maldonado, Sonora), and 'Crystallography Techniques in Clay Mineralogy' (R.W. Berry, California, and J. Ledesma, California), and workshops on 'Powder X-Ray diffractometry' (U. Preckwinkel, Wisconsin, G. Picco, Spectramex, and C. Duarte, Sonora), 'Crystallographic shapes for youngsters' (A. Cordero, UNAM) and 'SHELX97' (B. Stec, Texas, and R. Sotelo, Sonora) were run. A 'Lotto of the materials' for children was offered by P. Quintana (Yucatán). Students received course books. The exhibition featured new equipment and services from Bruker, Philips, Bede, Pona, Hitachi, and Spectramex. Additional information is available at www.unam.mx/smc. The congress was sponsored by the Education Dept of the Mexican Government (SEP), the Nat'l Council of Science and Technology (CONACyT), the Latinoamerican Centre of Physics (CLAF-Mexico), the Nat'l U. of Mexico (UNAM) and the SMCr. Crystallographers of Morelia City, in Michoacán, México, will host the congress in 2003.

Adolfo E. Cordero-Borboa, cordero@fisica.unam.mx

MEETING REPORT

Second Belgian symposium



Speakers at the Second Belgian Crystallography Symposium BCS-2. Left to right: A. Lucas, P. Launois, H. Zabel.

More than 100 scientists took part in the Second Belgian Crystallography Symposium BCS-2, which was held in October, 2001 at the Academy House, adjacent to the Royal Palace in Brussels. The Belgian Nat'l Committee for Crystallography organizes this symposium at biennial intervals to promote interdisciplinary contacts between Belgian scientists who use diffraction and microscopy techniques for atomic scale studies in the apparently unrelated fields of condensed matter chemistry and physics, material sciences, earth sciences and life sciences. As one of the main objectives was to promote personal contacts, plenary lectures were limited to three and given by distinguished colleagues in widely different fields: 'X-ray and electron diffraction by molecular helices' by A. Lucas (Namur), 'Fullerene compounds and nanotubes: X-ray scattering investigations' by P. Launois (Paris-Sud) and 'X-ray and neutron studies on thin films' by H. Zabel (Bochum). The 38 posters, grouped in four sections attracted much attention and discussion. The meeting was sponsored by both Royal Academies of Belgium for Science and the Arts, and the firms Bruker Belgium, Bruker Nonius, EFG Rigaku, MarResearch and Philips.

Luc Van Meervelt

MEETING REPORT

Guinier remembered



The annual Meeting of the French Crystallographic Assn was held in Orsay, on the campus of the U. Paris XI, in July 2001. The meeting began with a tribute to André Guinier, renowned physicist and crystallographer, who died on July 3, 2000 [see the obituary in *Acta Cryst.* (2001) **A57**, 1-3].

A. Guinier was a pioneer in the investigation of local order and disorder in condensed matter. He was one of the first to understand, demonstrate and exploit the richness of the information contained in both small-angle and wide-angle diffuse scattering phenomena. In small-angle diffuse scattering, his name is associated with the co-discovery of the Guinier-Preston zones (small clusters of atoms that form during precipitation in age-hardening alloys). Wide-angle diffuse scattering reveals positional, chemical or occupational partial order. The first session of the meeting was devoted to an illustration of such phenomena, with recent results obtained in polymers, liquid crystals, glasses, proteins and charge-density wave systems.

Guinier, a member of the French Academy of Sciences, also played an important role in promoting and organizing physical sciences at the national and international level (he had been President of the IUCr (1966-69)). These diverse activities were evoked in a session chaired by H. Curien, President of the French Academy of Sciences, a physicist and crystallographer himself.

Three plenary lectures were given. M. Verdaguer (Paris) explained the role of crystallography in understanding the structural cause of magnetism, the properties of molecular magnets and the design of new materials. P.M. Alzari (Paris) described one of the national programs of research in genomics, 'Structural genomics of mycobacteria', reviewed other national and international genomic programs and emphasized that important technological advances are revolutionizing this field. J. Baruchel (Grenoble) gave an overview of the spectacular progress made in X-ray imaging methods, including phase imaging, use of coherent beams, time resolved imaging or topo-tomography.

Two plenary sessions on 'Interfacial membranes' and 'New tools for x-ray synchrotron and neutron research' were chaired by J.-L. Popot, T. Zemb and C. Fermon, J. Susini, respectively.

The rest of the program was distributed among eight parallel sessions covering the topics of structural inorganic and mineral chemistry (D. Grébillé, chair), protein-protein interactions (M. Knossow, chair), artificial low-dimensional structures – interfaces (M. Sauvage-Simkin, chair), new methods for structural analysis in biology (A. Podjarny, chair), structural molecular and coordination chemistry (J.-C. Daran, chair), hot structures (M. Frey, chair), magnetism (B. Gillon, D. Givord, chairs), and structural pharmacology (J.-P. Samama, chair).

About 250 participants attended the Meeting organized by the French Crystallographic Assn and the Laboratoire de Physique des Solides in Orsay.

Roer Moret

MEETING REPORT

First Moroccan School of Crystallography



The faculty of sciences of Marrakesh organized the first school of Crystallography from January 29 – February 1, 2002. About 100 participants from Morocco, France, Spain, Italy and Netherlands took part in this school. The entire Moroccan university was represented by its teachers and young researchers. The IUCr and the European Crystallography Assn (ECA) were represented by their respective presidents Henk Schenk and Claude Lecomte who described the history, function and activities of the IUCr and the ECA and also presented talks.

Various topics were covered in the school including direct and reciprocal lattice theory, X-rays, electrons and neutrons diffraction and electron density analysis. N-dimensional crystallography and quasicrystals were taught by the pioneers of this discipline. Practical work sessions concerning the structure solution computer programs were organized during the school and recent diffraction equipments was described.

The school ended with a round table where the organizational committee described the state of crystallography in Morocco and noted the importance of the creation of the Moroccan Crystallography Association. The presidents of the IUCr and the ECA explained how the new Moroccan Association could join their organizations.

After the round table, the 80 Moroccan crystallographers coming from all the Moroccan universities approved unanimously the statutes of the AMC. An executive committee composed by 15 members was elected for 4 years as it's mentioned in the statutes.

Lecturers and topics included Single crystal diffraction (P. Becker, France); Crystal symmetry (M. Berraho, Morocco and A. Vegas, Spain); Electronic density (M.N. Bouhaida, Morocco), Direct and reciprocal lattices (A. Boukhari, Morocco); N-dimensional crystallography (M. Duneau, France); Examples of the structural resolution (L. EL Ammari, Morocco, A. Alvarez, Spain, and A. Boukhris, Morocco); Refinement of the structure and software presentation (N. Ghermani, France); Structure determination methods (C. Giacovazzo, Italy); Quasicrystals (D. Gratias, France); Powder Diffraction and Rietveld Method, (P. Gravereau, France); Data collection and reduction (M. Pierrot, France); and Electron diffraction (R. Portier, France)

Abdelmalek Thalal, Treasurer; AMC

MEETING REPORT

Crystallography in a castle



Participants at the 11th SOCC in August 2001.

An exquisite baroque castle in Rydzyna, Poland is the site of the triennial Int'l Organic Crystal Chemistry Symposia (SOCC). For the 11th SOCC, held in late August, 2001, the welcoming hosts were, as ever, the Chemistry staff of AMU, Posnan. This time chaired by T. Bonowiak. Polymorphism and intermolecular interactions were recurring themes in talks encompassing phase transformations, supramolecular structures, inclusion compounds and structure prediction, while many of the posters dealt with organic structures relevant to biological activity. The 70 participants came from a dozen countries, and IUCr support enabled young scientists from Moldava, Poland and Russia to present posters.

J. Karle, Honorary Chairman opened the Symposium with a retrospective view of attempts to explain the adhesion of molecules to form crystals, with a look forward to the computation of intermolecular interaction and packing energies in crystals in the 21st century. Later, D. Hofmann extended his systematic approach to structure prediction, utilizing the Flex Cryst program and the database of known structures. F. Allen noted that some so-called weak interactions such as non-H-mediated ones between C=O and C=N groups can approach hydrogen-bonding energies. Other accounts of the systematics of crystal structures came from V. Gorovov on energy calculations for hydrocarbons, V. Belsky on structural types of metal-halide crown-ether complexes, and L. Kuleshova on the high proportion of hydroxy compounds that form polysystem crystals in which molecules occupy more than one set of crystallographically independent positions.

Following an explanation by W. Hosseini of molecular tectonics, the structural design of supramolecular network formation, W. Jones described co-crystals in which organic guest molecules are intercolated in solid inorganic layers (his references to robust hosts, charged guests, and inserting guests between positively charged sheets were later quoted out of context). U. Rychlewska showed, with *ab initio* calculations, how dramatically molecule conformation can be influenced by the guest molecules in an inclusion compound. D. Braga reported that the organometallic dicarboxylic acid $[(N_5-C_5H_K COOH)_2 Co^{III}]$ is a versatile building block and forms crystalline halides and the co-crystal chloride monohydrate. W. Jankowski demonstrated the wide range of interaction in supramolecular structures.

After an introduction and illustration by C. Lecomte of the topological analysis of the charge density derived from synchrotron data, F. Larsen concentrated on low-temperature measurements to study short hydrogen bonds, M. Kubicki characterized weak intermolecular C-H hydrogen bonds by typological analysis, and A. Korlyukov discussed high-resolution X-ray diffraction for investigating hypervalency. H. Birkedal's study of polymorphism and stacking disorder recognized the presence of distant but closely similar monoclinic and hexagonal phases and interpreted diffuse scattering, as heavily faulted layer scattering. J. Meinnel utilized diffraction and inelastic scattering of neutron in his engagingly illustrated account of hindered rotation and tunneling of CH_3/CD_3 . Since circular birefringence has not normally been feasible in crystals in the presence of dominant linear birefringence, little is known about the orientational dependence of optical rotation in molecules. B. Kahr measured optical gyration in a low-symmetry MPH_4 isostructural series with an increasing polarizability [M=C, Si, Ge, Sn, Pb] and he showed beautiful illustrations of an investigation of the absorption energetics of inclusion overgrowth of dyes on facets of potassium sulfate crystals. M. Gdaniec utilized cholic acid and deoxycholic acid as chiral host materials wherein circular dichroism can be generated from organic guest molecules that are otherwise optically inactive and the helicity chromophores could be correlated with the Cotton effect.

Accounts of novel organic materials included reports of polymorphism in substituted pyridinium salts with potentially non-linear optical properties by T. Timofeeva, of ferromagnetic and antiferromagnetic systems by F. Iwnski, and of transitions between crystalline and rotator phases of long-chain ($n=17-24$) pure alkanes and their solid solutions and mixtures up to $n=37$ by S. Chazhengina.

W. Duax recounted the novel interactions of ions of the alternating d/l peptide gramicidin and water with the peptide framework in 25 Å long single file channels and coordination of cations with π -orbitals of C=O groups and peptide bonds in the channel wall. I. Karle described the design and self-assembly of hybrid peptides to form pores and tubules. For peptides with as many as 20 CH_2 groups in a chain, lipophilic guest molecules as large as pyrene and perylene can be solubilized within hydrophobic cavities.

Studies linking structure with biological or physiological activity included investigating the antimycotic activity of condensation products of salicylaldehyde (Yu Chumakov, Moldova), high-pressure effects on paracetamol polymorphs (E. Bolderova, Russia), the conformation of a $\text{CH}_2\text{-X}$ spacer between two pharmacophores in 2-substituted phenyl benzoxazoles (R. Czykowski), salts of O-phosphoryl-threonine, relevant to incorporation of phosphates in hormonal proteins (I. Bryndal), and channel solvates potential psychotropic activity (L. Mazur).

Cultured social activities (including a bonfire with beer and songs) within the castle and grounds balanced a full scientific program. As with recent SOCC, selected papers are to be published in a special issue of *J. Molecular Structure*.

Derry W. Jones

MEETING REPORT

Erice 2002



ECM20 reception in the courtyard of the oldest building of the Zagiellonon University where Copernicus studied.

The 32nd Erice course in Crystal Engineering entitled *Strength from Weakness: Structural Consequences of Weak Interaction in Molecules, Supramolecules and Crystals* emphasized the study of interactions not just by crystallography, but also by techniques ranging from gas phase electron diffraction, IR and NMR to theoretical techniques. Important points were raised about the meaningfulness of comparing measurement of parameters obtained by different techniques, given the fact that different techniques measure different things. Sometimes there is an obvious difference such as the difference between a time averaged structure and a single 'freeze frame' snap shot of a molecule in motion or the differences between theoretical calculations calculated for an idealized case at absolute zero and experimental results obtained at ambient temperatures for a molecule in a real system. The highlight of the meeting was the lively, (sometimes heated!) debates on the nature of hydrogen bonds, especially the existence of 'blue shifted hydrogen bonds' (Hobza) and the classification of strong hydrogen bonds (Gilli), and on the virtues or otherwise of theoretical *versus* experimental techniques.

Charlotte Broder, U. of Durham

MEETING REPORT

International ferroelectrics

At the previous European ferroelectric meeting, the emphasis was on phase transitions. At the most recent meeting in September, 2001, in Madrid, the topics were much more diverse, with interest in thin films and other areas gaining in significance. Ferroelectric smart cards are already a 2.5 billion dollar industry and non-volatile ferroelectric memories are on the market. Prof. Ginzburg placed phase transitions in ferroelectrics in historical context and emphasized the importance of toroidal moment. Prof. Muller, the 1987 Nobel Prize winner, spoke about tricritical points and incommensurate phases. Some presentations of Particular interest concerned: A 2-dimensional Ising-like model for ferroelectric behavior (A. Garcia), the atomistic mechanism in relaxor ferroelectrics (T. Egami), the use of Raman spectroscopy to measure complete dispersion curves (P. Baranek), the importance of coupling between the modes for the soft mode phase transition (S. Kamba) and K. Parlinski's 'phonon' program,

Wednesday morning consisted of very enlightening talks about great 20th Century Solid State Physicists', including the Braggs (A. M. Glazer), Peter Debye (E. Courten) and Landau (V. Ginzburg).

Vincent Jennings, U. of Warwick

MEETING REPORT

Dutch Workgroup on Powder Diffraction

In 1988 the Workgroup on Powder Diffraction (WPD) of the Dutch Crystallographic Assn (NVK) was founded in order to exchange information about the functionality and availability of powder diffraction software, and to develop standardization of data formats. Because no easily accessible well-developed powder diffraction database was available, the Dutch WPD decided to start a database. For lack of money and because of the improved availability of software via the WWW the Dutch WPD stopped this activity which was taken over by the Information Exchange Bank.

The Dutch WPD advocated adopting the JCAMP-DX format as a standard in powder diffraction, however, CIF format has become the standard. The Dutch WPD is currently participating in a project for the standardisation of powder diffraction methods of CEN, the European committee for the development of standards. In an *ad hoc* group representatives of several European countries write standard procedures to measure and evaluate powder diffraction data.

The Dutch WPD organizes powder diffraction meetings and contributed to the organization of EPDIC-2 in Enschede in 1992. Since 1991, a biennial (every other year) one-day meeting is organised for Dutch speaking powder diffractionists.

On the 12th anniversary of the founding of the Dutch WPD a meeting was held on March 23, 2001 at the U. of Utrecht. Speakers focused on the development of X-ray optics and hardware during the last decade. Topics included the future of powder diffraction in the Netherlands (R. Delhez, TUD), optical elements in powder diffraction (C. Reiss, Philips Analytical B.V.), the applicability of 2-dimensional detectors in powder diffraction (E. Hovestreyd, Bruker), micro and macro X-ray sources (F. van Meurs, Nonius), the possibilities of a synchrotron (H. Graafsma, ESRF), and the capabilities of the X'celerator, a new fast linear X-ray detector (M. Fransen, Philips Analytical B.V.). Technical developments of the last decade are opening new fields and the WPD plans to continue its support to the Dutch powder diffraction community to explore new opportunities.

Roelie Olthof-Hazekamp

Sec. Nat'l Committee Crystallography, Netherlands

MEETING REPORT

Collective Action for Nomadic Small-angle Scatterers (canSAS-3)



Els Homan explains the integrated acquisition and pre-processing for the DUBBLE beamline.

The aims of the canSAS meetings are to promote and simplify the sharing of SAS data analysis methods. The third workshop held at the ILL in May, 2001 attracted 30 participants. The workshop organized by the ILL, EMBL, ESRF and the DUBBLE-CRG brought together practitioners at the leading edge of data analysis and computer scientists working on advanced data storage techniques.

The disparity in data formats triggered the first canSAS meeting in 1998. In opening canSAS-3, W. Bras (DUBBLECRG) stressed the need for merging SAS data from different instruments and facilities and called for cooperation on writing data for simple measurements. High intensity instruments have brought significant increases in complex measurements, with time-dependent 2D data sets exceeding several Gigabytes.

J. Barnes (NIST) stressed the need to conserve a maximum number of parameters (meta-data) including error estimates. The Neutron and X-ray communities are promoting NeXus, a self-describing data format, based on the NCSA Hierarchical Data Format (HDF). To allow the use of simple ASCII files, the sasCIF format, an extension of the Crystallographic Information File (CIF) was written by D. Svergun and M. Malfois (DUBBLE-CRG) who reported recent modifications. S. King (ISIS) identified additional meta-data required for Time of Flight (TOF) neutron data. Marc's document matching sasCIF names and NeXus meta-data names was well received. R. Ghosh (ILL) described efforts to introduce XML, a rapidly developing standard for data interchange, as a wrapper for the multifarious file formats presently in use. There was general recognition that XML might well offer procedures for progressively introducing a WWW based definition of 1D data and meta-data. L. Gilbertson (ILL) demonstrated how a short Python script offered easy access to XML files, driven from a simple GUI. E. Pourmel (NCSA) described the Hierarchical Data File developed at the NCSA. Version 4 had been adopted by the NeXus development group for storage of raw data. The demonstrations of browsers with editing features, H5-View (E. Pourmel), and good graphics (E. Boucher, APS) convinced those present that HDF-5 should be adopted for complex data storage. U. Filge (PSI) described a new version of NeXus based on HDF-5.

P. Besecke (ESRF) described the problems encountered in merging SAXS and WAXS data and of the distortions arising as the WAXS detector is rotated about the sample. Since new SANS instruments are likely to be on pulsed sources, dealing with TOFSANS is of major interest. E. Litvinenko (JINR) demonstrated how PV-WAVE displays and evaluates TOF-SANS data. This is essential for examining graphically various data quality indicators. R. Hjelm (LANSCE) showed how the data quality could be defined before performing final data reduction of TOF-SANS. He had chosen HDF/NeXus as a data format since it offered the best means for storing the complex raw data.

The packages which have been used for SAS analysis include PV-WAVE, IDL, MATLAB, IGOR, OCTAVE, as well as maintained programs such as FIT2D. Common dependencies on X-window (Unix) or PC-Windows have been resolved, and the user sees the same interface on either type of platform. The primary

attraction in using packages is that the aspect of computer platform independence is resolved by the package authors.

A. Munter (NIST) described the system at NIST which is based on IGOR, but expressed reluctant to continue development. C. Dewhurst (ILL) demonstrated GRASP, based on MATLAB. This includes many automatic features for matching data taken in different instrument configurations, as well as 2D fitting etc. The easy ability to compile and freely distribute MATLAB executables is an exception for commercial packages. E. Homan (EMBL) demonstrated the integrated control and treatment software developed using IDL for the DUBBLE-CRG SAXS-WAXS beamline at the ESRF. Andy Hammersley (ESRF) showed that his FIT2D includes calibration corrections needed for high precision work. Although based on a GUI, he wonders whether such products could benefit from a macro language (perhaps Python based) for repetitive operations. M. Rodman, (SRS, Daresbury) described GraphApp, a GUI C library, which enables applications to be compiled either on PC-Windows, or X-window. This allows stand-alone executables to be created.

The session devoted to applications included fibre diffraction, biological molecules in solution, super-alloys, and rope. T. Forsyth (ILL) presented his study of polymorphism in DNA. D. Svergun's (EMBL) programs can ignore meta-data and hunt for tables of intensity-Q values.

Problems of measuring weak signals were raised by A. Rennie (King's College, London). When backgrounds are high the propagation of errors is needed in assessing final results. With complex samples such as fibres, the SAS diffraction geometry requires correction before interpretation of the 2D SANS diffraction patterns. He reported success in matching results at different facilities using distinct program suites. A new challenge was posed by high-fluxes, where on-line analysis had to be developed to follow complex measurements.

The activists in Grenoble, Didcot and Washington proposed continued exchange of examples of XML data files; all agreed to look at the possibilities of using HDF-5 utilities to construct sample data files of complex measurements as examples to display in Venice at SAS-2002.

There was general agreement that canSAS should serve as a forum for debating analysis techniques and disseminating information on programs and should create a website dedicated to these aims.

R. Ghosh, ILL, C. Ferrero, ESRF, Grenoble, October 2001

MEETING REPORT

Computing and teaching microsymbiosia at ECM20



Controversial session on software solutions at ECM20.

A Microsymposia on the contemporary topic of Computing and Teaching featured six speakers who delighted the audience with a wide range of topics on using the Internet for distance learning, virtual courses in crystallography and various models for delivery of curriculum. Some key issues regarding the pace of introducing new technologies, the role of government in delivering mass education and the pressures on institutions in responding to the novel methods of education was raised during the talks. Y. Epelboin (CNRS, Paris) [1] in the opening address asked, 'What can we learn from actual experience?' and compared the US experience with the European paradigm. He projected that the world education market [2] by 2002 would be worth an estimated 90 billion US dollars. Distance learning would open up the accessibility to virtual documents and libraries facilitating politicians to contain the budget for education. However, the case was argued that the rich diverse tapestry of language and traditions that is European culture could not so easily be swayed by an economic model. Cooperation via Brussels would ensure that the 'Revolution would go marching on.' Was the idiosyncratic Gallic rally.

At the heart of G. Chapuis' talk (Lausanne, Switzerland) was the 'nuts and bolts' of implementing interactive web applications of Java applets to provide simulation of some key crystallographic concepts. He listed the ingredients for a virtual course in crystallography concentrating on the tools for simulation and provided a number of real time demonstrations of the Ewald sphere, Laue pattern diagrams and Fourier transforms. The didactic road is long to a complete course on the Internet although within a Java environment using a web browser simulations can be performed, directly independent of the computer platform being used. This time the baton was passed on to the IUCr to promote and establish structured learning modules for potential crystallography students. C. Sansom (Birbeck, London) described at length the Masters level distance learning courses in Structural Biology offered by Birbeck College since 1996. She gave an overview profile of the average student taking the course as mature with demanding professional careers quipping 'that there were no typical students'. The communication links between students and teachers were maintained using a purpose built Internet chat room or MUD for short (multi-user Dimension). Much of the material is written in simple HTML, which can be run on a low specification computer, course material being made available at regular intervals throughout the year. It was stressed that fees were kept low to encourage wide student participation in the Advanced certificate on the Principles of Protein Structure (PPS) [4].

The first of two talks on powder diffraction commenced with A. Le Bail (U. du Maine, France) who challenged the audience to think 'where is all the knowledge.' And reminded us that distance learning was in its centenary. The dangers of online education are well established [5] with the automation of Higher Education likened to creating 'Digital diploma mills' as the pervasive new information technologies advance. The provision of a powder diffraction course was inspired by the Birbeck model and the speaker emphasized the deliberation in choosing between a synchrotronous and asynchrotronous mode of learning. The course material with pedagogic exercises is available on Structure Determination by Powder Diffractometry (SSPD) [6] and can be viewed on the web. Caution

was advised that expert systems could kill the interest of deep learning and that an explosion of software diversity could pose a nightmare for student and teacher alike.

The compatibility of the Powder Diffraction on the Web course [7] with both Netscape and Internet Explorer 3 was mentioned as well as being Java/Java script free. As it is easy 'to get lost in hyperspace' the material makes extensive use of course navigation buttons on the web pages. The material itself is organized into three areas; experimental methods covering basic crystallography, diffraction and symmetry, data analysis covering both quantitative and qualitative aspects and a project on Rietveld refinement.

Reference:

- [1] <http://www.lmcp.jussieu.fr/~epelboin>
- [2] <http://www.wemex.com>
- [3] Chapuis G. & Hardaker W., *J. Appl. Cryst.* (1999) 32, 1164-1168
- [4] <http://www.cryst.bbl.ac.uk/pps/index.html>
- [5] Nobel D. – <http://www.communication.ucsd.edu/dl>
- [6] <http://sdpd.univ-lemans.fr/course/index.html>
- [7] <http://pd.cryst.bbk.ac.uk/pd/welcome.htm>

Jim Kelly, Industrial Materials Group, School of Crystallography, Birkbeck College

MEETING REPORT

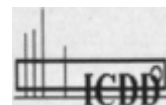
BCA Pharmaceutical Group

Paul Higginson of Pfizer opened the meeting in June, 2001 at Glaxo-Smith-Klien with 'Automated Solutions to High Throughput Crystal Screening'. In her presentation on 'Prediction, Morphology and Mechanical Properties of Paracetamol', S. Price of UCL demonstrated how difficult polymorph prediction can be, and described ways that may make it feasible in the future. C. Anderston described 'On-Line Monitoring of Solid-State Form during Crystallizations by Raman Spectroscopy', and A. van Langevelde of Crystallics, a company which specializes in polymorph characterization. discussed 'High Throughput XRPD in Polymorph Discovery' in 'DASHtastic Adventures of the Bruker-D8' A. Florence described solving molecular structures from Powder diffraction data. D. Beckers (Phillips Analytical) discussed unexpected phase transition at high temperature or humidity during storage or transport that can turn a powerful medicine into a useless powder. C. Weston of Bruker AXS outlined 'X-ray Rapid Screening System for Combinatorial Chemistry'.

Brett Cooper and Neil Feeder, from BCA Crystallography News, No. 78, Sept 2001

AWARDS AND PRIZES

2002 Ludo Frevel Crystallography Scholarships



The ICDD Ludo Frevel Crystallography Scholarship Committee has selected six recipients for the 2002 Scholarship program. These recipients were selected, on a competitive basis, from forty-one well deserving applications received by the ICDD Scholarship Committee. The recipients are:

Dane A. Boysen (California Inst. of Technology, Pasadena, CA) with research involving 'Hydrogen-Bonding, Phase Transitions, and Proton Conductivity in MH_2PO_4 -Type Solid Acids ($\text{M}=\text{Li}, \text{K}, \text{Na}, \text{Rb}, \text{Cs}$ and NH_4);' **Desiree H. Fong** (McGill U., Montreal, Quebec, Canada) with exploration into 'Structural Analysis of an Antibiotic-Detoxifying Kinase;' **Jeffrey H. Haeni** (Pennsylvania State U., University Park, PA) with major interest in 'Growth and Characterization of Metastable $\text{BaTiO}_3/\text{SrTiO}_3$ Superlattices;' **Michael W. Lufaso** (Ohio State U., Columbus, OH) with studies focusing on 'Evaluation and Prediction of the Crystal Structures of Single/Ordered/Disordered Octahedral Cation Perovskites Using the Software Program SPuDS;' **Jeffrey P. Maranchi** (Carnegie Mellon U., Pittsburgh, PA) with research concerning 'Novel Chemical Synthesis and Characterization of Electrode Materials for Thin Film Lithium-Ion Batteries;' and **Christine M. Clark McCracken** (U. of Manitoba, Winnipeg, Manitoba, Canada) who's investigating 'The Crystallography and Chemistry of Tourmaline.'

The ICDD will present each of these students with a check in the amount of \$2,250, to help them continue their studies in their selected fields of crystallographic research.

Helen M. McDonnell

MISCELLANY

Ladies Beware

Ladies beware if you are invited to go for a walk with Henk Schenk on a Sunday afternoon on the sand dunes along the coast north west of Amsterdam. You might come back with quartets.

(See [Letter from the President](#), IUCr Newsletter 9(2) page 1)

Howard Flack

AWARDS AND PRIZES

Congratulations...

• The \$35,000 Minister's Prize for Achievement in Life Sciences has been awarded to **Bostjan Kobe** of the U. of Queensland for research in exploring the shape of basic building blocks-proteins. The Prime Minister and Minister for Industry, Science and Resources presented the 2001 Science Prizes to the winner during a dinner in the Great Hall of Parliament House on September 25 2001.

• **Arjen van Langevelde** was awarded the DOW Energy Dissertation Prize for his thesis 'Triglycerol structures and the Cocoa-butter Crystallisation'. His work leads to a new way of producing chocolate which uses less energy as the usual production processes. He prepared his thesis in Henk Schenk's group at the U. of Amsterdam.

• **Julie Goodfellow** from Birkbeck College, U. of London, will become one of the first women to head one of the British Government's seven scientific Research Councils. Her research interests include the use of computer simulation techniques to study the structure and function of large molecules.

• **Graeme Davies** has succeeded Brian Eyre as Chair of the Council for the Central Laboratory of the Research Councils (CCLRC).

• **Raymond P. Goehner** and **Joseph R. Michael**, both of Sandia Nat'l Laboratories, Albuquerque, NM, receive the 2001 J.D. Hanawalt Award for excellence in the field of X-Ray Powder Diffraction. Goehner and Michael presented the Hanawalt Award Lecture entitled, 'Phase Identification Using Electron Backscatter Diffraction in the SEM: A Powerful Tool for Materials Science' at the 50th Annual Denver X-Ray Conference in Steamboat Springs, CO, USA, August 1, 2001. Previous recipients of the prestigious award include: Herbert Gobel, 1998; Daniel Louer, 1992; William Parrish, 1986; and Ludo K. Frevel, 1983.

• **James Watson**, co-discoverer with Francis Crick, of the double-helix structure of DNA, has received an honorary knighthood for 'services to the UK-American partnership in the field of genetics and science'. Watson is president of the Cold Spring Harbor Laboratory.

• **Stephen Z. Goldberg**, (Prof. of Chemistry, Adelphi U., NY) is one of ten newly elected members of the American Assn of University Professors (AAUP) National Council (Washington, D.C.).

• **Winnie Wong-Ng** (NIST, Gaithersburg, MD) was elected as a Fellow of the American Ceramics Society recently 'For recognition of the notable contributions to the Ceramic Arts and Sciences'.

• In May 2001, **Jeanette Krause Bauer** was awarded the U. of Cincinnati McMicken Excellence Award. Since coming to Cincinnati, she has increased, by six times, the number of structures determined annually by the UC facility. Jeanette has organized the 59th Pittsburgh Diffraction conference, and she will serve as the Program Chair of the ACA 2003 National Meeting.

• Inst. of Medicine (IOM), part of the National Academies elects new Member **Gregory A. Petsko**, Gyula & Katica Tauber Prof. of Biochemistry & Chemistry, and director, Rosenstiel Basic Medical Sciences Research Center, Brandeis U., Waltham, MA.

• **Wade Adams**, former chief scientist at the Air Force Research Laboratory (AFRL), Materials and Manufacturing Directorate, at Wright-Patterson Air Force Base in Dayton, OH, became the new director of the Center for Nanoscale Science and Technology (CNST) at Rice U. in January.

NOTICE

Nene, Nana, Nano

A US Dept of Energy (DOE) report entitled 'Complex System, Science for the 21st Century' predicts the next millenium will take us into the world of complexity in which the disciplines of physics, chemistry, material science and biology will converge. Crystallography has always been at that convergence point as the programs of the IUCr Congress demonstrate. 'Nanoscale Science, Engineering and Technology Research Direction' another DOE report, calls for greatly expanded long term support because Nanoscale Technology will be a strategic branch of science and engineering for the next century, one that will fundamentally restructure technology currently used for manufacturing medicine, defense, environmental management, energy production, transportation, communication, computation and education. Since Nanotechnology involves the control of matter at the atomic or molecular level, crystal structure determination provides some of the most reliable information possible with which to understand these processes.

(No matter what you rename it, it is still structure and function.)-Ed.

NOTICE

Human rights

The American Assn for the Advancement of Science (AAAS) sent a letter to the US State Dept. complaining of human rights abuses in the treatment of Wen Ho Lee that might deter foreign students from studying in the U.S. Incensed by a presidential decree to conduct more routine polygraphs in defense laboratories, the National Academy of Sciences (NAS) initiated a study to investigate the validity of polygraphs. Similarly intrusive is the 1996 act of US Congress to develop an Internet-based system to track foreign students working on projects considered sensitive. The AAAS is working on the repeal of the entire system.

The importance of scientists' rights to travel was raised with emphasis on relations with Cuba. AAAS representatives had visited Cuba with the hope of improving exchange. A survey can be found at <http://shr.aaas.org/rtt>.

NOTICE

A whopper of a carbon-carbon bond

Carbon-Carbon bonds that are 2.9 Å or longer have been identified in a small class of electron-transfer salts. Of these salts, cations assist pairs of tetracyanoethylene (TCNE) radical anions to overcome their electrostatic repulsion and form unusually long bonds between the ethylene carbons of two neighboring TCNE anions. These weak, elongated bonds, created by overlap of two singly occupied π^* orbitals, involve four carbon atoms sharing two electrons.

C & EN/July 9, 2001

AWARDS AND PRIZES

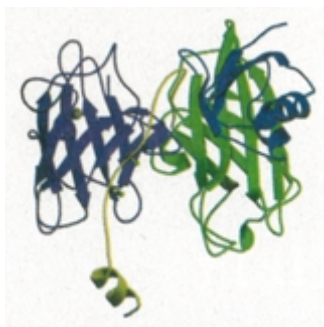
CCDC Chemical Crystallography Prize for Younger Scientists

Nominations are invited for this award, to be made at the BCA Spring 2002 Meeting. The award is sponsored by the Cambridge Crystallographic Data Centre. The award is for original research in the field of chemical crystallography or the application of crystallographic information to structural chemistry.

Further details and a nomination form may be obtained from the Secretary of the Chemical Crystallography Group, H.R. Powell, hrp1000@cam.ac.uk

NOTICE

Metal chaperones at work



Audry L. Lamb and Amy C. Rosenzweig have determined the x-ray structure of a chaperone protein that transports copper, complexed with its target enzyme, a super-oxide dismutase called SOD1 [*Nat. Struct. Biol.*, **8**,751 (2001)]. 'We have the first image of a structure that delivers copper to its target,' Lamb says.

Rebecca Rawls

from C&EN/September 10, 2001

REGIONAL NEWS

British Crystallographic Assn



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Vice President: P. Fewster

Secretary: C. Cardin

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<http://gordon.cryst.bbk.ac.uk/BCA/index.html>

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Vice President: B. Ali

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Assessors: A. Jilali, B. Aïcha, B. Abdellah, E.Q.S. Eddine, E. Abdelaaziz, M. Idriss, M. Bouchaïb, N. Abdelilah, R. Mohamed, S. Ismael, Z. Driss

European Crystallographic Assn



Executive Committee

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Secretary: G. Filippini

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Members: E.J. Dodson, M. Jaskolski, D. Viterbo

www.ecanews.org

American Crystallographic Assn



Council Officers 2002

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Vice President: R.E. Davis

Past President: W.C. Stallings

Treasurer: D. Ohlendorf

Secretary: L. Brammer

www.hwi.buffalo.edu/ACA/

News Editors

BCA Crystallographic News: R. Gould (U. of Edinburgh)

ACA Newsletter: C. Chidester, J. Flippen Anderson (Naval Research Labs)

AWARDS AND PRIZES

Ewald Prize

The IUCr is pleased to announce that Professor Michael M. Woolfson has been awarded the sixth Ewald Prize for his exceptional contributions in developing the conceptual and theoretical framework of direct methods along with the algorithm design and computer programs for automatic solutions that changed the face of structural science and for his contributions to crystallographic education and international collaboration, which have strengthened the intellectual development of crystallographers worldwide.

The presentation of the Ewald Prize will be made during the Geneva Congress Opening Ceremony on Aug. 6, 2002.

AWARDS AND PRIZES

The Jeffrey Award call for applications

A fund established in memory of George A. Jeffrey will be used to assist outstanding students to attend the Congresses of the IUCr. The first award(s) will be made at the Geneva Congress. Applications are invited worldwide. These must be from graduate students in good standing at the time of the Congress.

Applications must include: A one-page letter explaining the student's background and any special circumstances in support of the application. Letters of recommendation from the student's mentor and from one other person familiar with the student's crystallographic abilities and background. The mentor should state the expected date for the student's graduation. A one-page biographical sketch of the student. Copies of any reprints, preprints or abstracts in which the student is an author. An abstract with the student as first author, which has been submitted for the program of the Geneva Congress. The student's e-mail address.

The original and two copies of the application (in English) should be mailed to: B. Craven, Chemistry Dept, Indiana U. of Pennsylvania, Indiana, PA 15732, USA. It must be received no later than May 15, 2002. Applications will be judged by B. Craven, H. Berman (Rutgers U.) and M. Caffrey (Ohio State U.). The important criteria will be the scientific excellence of the student's research, the student's financial need and the student's proficiency in English, the official language of the Congress. The Jeffrey Award will cover at least the student's registration fee and the cost of student housing.

OBITUARY

Max Perutz (1914-2002)



Sketch by Julia Duax

Early on Wednesday, February 6, Max Perutz died of cancer after a long and productive life. Starting a Ph.D. in 1936 under J.D. Bernal at the Cavendish Laboratory, he applied X-ray crystallography to proteins and in 1953 developed the method of isomorphous replacement using heavy atoms to solve the phase problem. This led to the solution of the first protein structures, those of myoglobin by his colleague John Kendrew and his collaborators, and of haemoglobin by Perutz and his collaborators. For this, Perutz and Kendrew were awarded the 1962 Nobel Prize for Chemistry. With a great deal more work during the 1960's, Perutz and his colleagues went on to solve the atomic structures of both oxy- and deoxy-haemoglobin which allowed him to propose a stereochemical mechanism for the cooperative binding of oxygen to haemoglobin. Max was the first author of a recent review (*Ann. Rev. Biophysics and Biomolecular Structure* 1998) of cooperativity in haemoglobin in which he noted that his mechanism still appeared to be correct.

In more recent years, he worked on ligand binding to haemoglobin to help develop a clinically useful drug for increasing oxygen delivery to hypoxic tumours for radiation therapy, and to infarcted tissues. He also developed a strong interest in the structure of the polyglutamine tracts in Huntington's disease. In his youth, as a sideline, he also worked on glaciers. He studied the transformation of snowflakes that fall on glaciers into the huge single ice crystals that make up its bulk, and the relationship between the mechanical properties of ice measured in the laboratory and the mechanism of glacier flow. He was a prolific and talented writer of popular articles and book reviews, many published in the *New York Review of Books*. He also wrote a number of books, including 'Is Science Necessary' and 'I wish I'd made you angry earlier' which are collections of essays. 'Science is not a quiet Life' published by World Scientific Publishing is essentially his scientific autobiography.



The porphyrin molecule in hemoglobin. (provided by Anthony Addlagatta)

At the Cavendish Laboratory with the support of Prof. Lawrence Bragg and with his first Ph.D. student, John Kendrew, who joined him in 1945, he built up a group working on the molecular structure of biological systems which grew to four people in 1950 and to about 40 people by 1960. Merging then with other groups from Cambridge and London to create the MRC Laboratory of Molecular Biology on the Hills Road site (now Addenbrooke's) in 1962, he became Chairman of the new Laboratory until 1979 when he 'retired'. Since then he has worked nearly every day in the Laboratory which has grown to house over 400 people. Over the years, the Laboratory has been a prolific source of discoveries and inventions. In addition to his own research achievements, Max will be remembered for his interest in and warm support of the work of others, and as one of the founders of Molecular Biology

London Times, 2/7/02, www2.mrc-lmb.cam.ac.uk/Max_Perutz.html

OBITUARY

Robert A. Sparks (1928-2001)

Bob Sparks died July 29, 2001 at the age of 72, in a car accident near Tillamook, Oregon. The accident also claimed the life of his beloved wife Nonie. Bob was born August 16, 1928 in Hollywood, California. He received his undergraduate and doctoral degrees at UCLA. He was a pioneer in the use of digital computers for crystallography, beginning with the Nat'l Bureau of Standards Western Automatic Computer (SWAC), one of the world's first digital computers, running it at night for crystallographic calculations and replacing the vacuum tubes one by one as they burned out. He worked on SWAC during the 1950's with his advisor, Prof. Kenneth Trueblood, and was proud to be co-author on several papers with Dorothy Crowfoot Hodgkin for three-dimensional Fourier calculations on SWAC to solve the hexacarboxylic acid derivative structure of vitamin B₁₂, the largest structure of that time. Following his Ph.D. he was a postdoctoral fellow with Dr. Hodgkin at Oxford U. He served in the US Quartermaster Corps during the Korean War, where as Bob wryly recounted, the army chose to use his skills testing plastic trays for durability instead of continuing his collaboration programming of the 'Giant Brain' at Los Alamos Scientific Laboratory. At IBM Research in New York in 1960 he co-published with Peter Gantzel and Ken Trueblood the UCLA Structure Factor Least Squares program. He was the founding director of the Statistical and Computing Center at the U. of Hawaii before returning to California to become Director of Research Information and Data Processing at Syntex Research, 1965-1969. Bob returned to his Crystallographic roots, co-founding Syntex Analytical Instruments to develop and manufacture computer-controlled single-crystal diffractometers. This set the course for the rest of his career, as Bob remained a driving force behind the development of four-circle and CCD diffractometers for Syntex, Nicolet, Siemens, and finally Bruker Nonius. He served as ACA treasurer from 1980 to 1985. With Ken Trueblood, he developed a national course for teaching crystallography. In 1998 he received an ACA public service award for his teaching. In 1978 he founded California Scientific Systems (CSS) with A. Christensen and S.K. Byram, to develop and manufacture powder diffraction software and automation systems. CSS was acquired in 1982 by Nicolet. His untimely death brought many messages which praised his vast and understated knowledge, his infectious enthusiasm, his patience with everyone willing to learn, and his drive to pursue his vision of what was right for crystallography. Professional dedications to him include the twinning workshop at ECM 2001, sessions at the Pittsburgh Diffraction Conference 2001 and the ACA-San Antonio 2002, and a tribute in Madison at Bruker AXS.

Susan K. Byram

OBITUARY

Richard K. McMullan (1929-2002)



Richard McMullan died of heart failure on March 2 during his sleep. In the twenty years up to his retirement in 1994, he was a staff member in the Chemistry Dept at the Brookhaven National Laboratory. There he did much to develop the neutron diffraction facilities for chemical crystallography. This included the writing of diffractometer software, the design of vacuum systems for crystallizing gases and unstable compounds and the building of cryostats and furnaces for neutron data collection at temperatures from 15K to 1500K. These facilities formed the basis for his many collaborations with other Brookhaven staff and a multitude of visitors who came from all over the world. Dick's modesty, patience, enthusiasm and dedication to the highest scientific standards were well known to all those who had the benefit of his friendship and partnership.

In 1956, Dick obtained his PhD at Iowa State U. in inorganic chemistry. He came to the U. of Pittsburgh in 1958 in order to take up X-ray crystallography. There, he joined G.A. Jeffrey and his group and spent a decade in systematic studies of a series of intricate clathrate hydrates, notably those with alkylammonium and sulfonium salts as guests. During 1967-69, Dick was in Germany as a Humboldt Visiting Fellow working with Professors Mootz and Saenger on the structures of *cyclo*-dextrin complexes. From then until his move to Brookhaven, he was with Prof. Sundaralingam at the U. of Wisconsin, working on the structure of *t*-RNA.

His life style was very frugal. He once said that all his worldly possessions could be packed into his beloved Buick. His hospitality was famous. Visitors thronged to his apartment, often as many as six crowded for dinner around his tiny table (23" wide, 35" long, flaps up). Usually it was a visitor who cooked up some specialty from far away. All was noise and merriment until about 10pm when Dick would announce it was time to go back to the reactor.

When it was decided to hold a Pittsburgh Diffraction Conference in honor of his retirement, I was advised that preparations needed to be well beyond the point of no return before informing Dick. Otherwise he might well decline to attend. In fact, I believe he was delighted. He made only one condition, namely that he would not have to give a speech. However, at the conference dinner, after so many had paid tribute to him, Dick found himself on his feet speaking easily and warmly in response.

Bryan Craven

OBITUARY

Sten Samson (1916-2001)

Sten Samson passed away on November, 17 2001, after a short illness. He was 85 years old. Sten received his Fil. kand. degree at the U. of Stockholm in 1953 and came to the California Inst. of Technology to work with Linus Pauling on the structures of intermetallic compounds. He returned to Stockholm in 1956 and obtained his Fil. lic. Degree in 1957; he then returned to Caltech for the remainder of his career. He was granted a Fil. dr. degree from the U. of Stockholm in 1968.

Sten was widely known because of his ability to understand the structural principles governing very complicated intermetallic compounds, and his knack for designing and constructing innovative x-ray diffraction equipment. Several commercial models of serial diffractometers included Stens design features, particularly helium cryostat versions capable of operating below 20 K which are in operation today. In the field of intermetallic compounds, his insight into coordination polyhedra and the ways in which they might pack together led to his discoveries of the structures of such compounds as 'NaCd₂', which has approximately 1200 atoms in the cubic unit cell. He was working on a further refinement of this structure (which is extensively disordered) until a short time before his death.

Sten is survived by a son, Karl, living in Stockholm, and a daughter Karin Lamar and two grandchildren, living in Colorado, USA.

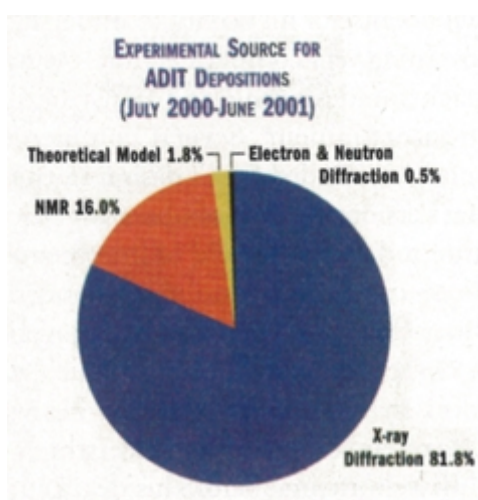
Dick Marsh

FEATURE ARTICLE

PDB Annual Report 2001



The PDB was founded in 1971 as the international repository for three-dimensional structure data of biological macromolecules. The PDB processes, stores, and disseminates structural coordinates and related information about proteins, nucleic acids, carbohydrates, and protein-nucleic acid complexes. The resource distributes information about all aspects of structural biology, including structural genomics, data representation formats, software, and educational materials. Currently in an average month, approximately 260 structures are deposited, 200 structures are released, and 2.6 million files of individual structure entries are downloaded from the PDB. The PDB's Data Uniformity Project enhances the consistency of existing (legacy) entries and maintains a consistent method of annotating current depositions.

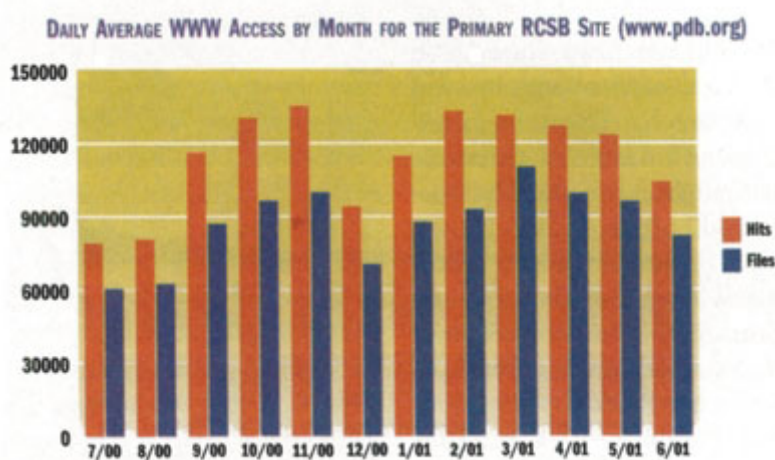


All legacy PDB entries and the recent RCSB entries are available in mmCIF format from the PDB beta FTP site at <ftp://beta.rcsb.org/pub/pdb/uniformity/data/mmcif/>. The files follow the latest version of the mmCIF dictionary supplemented by an exchange dictionary developed by the PDB and the EBI. This exchange dictionary can be obtained from <http://deposit.pdb.org/mmcif/>. An application program called CIFTr was made available for translating files in mmCIF format into files in PDB format. CIFTr works on UNIX platforms, and can be downloaded at <http://deposit.pdb.org/software/> (see below for more information).

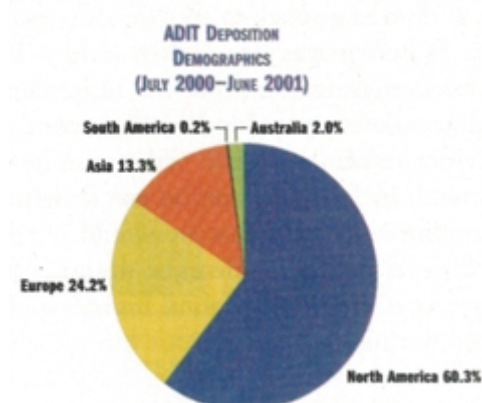
PDB HOLDINGS AS OF JUNE 30, 2001					
EXPERIMENTAL TECHNIQUE	MOLECULE TYPE				TOTAL
	PROTEINS, PEPTIDES, AND VIRUSES	PROTEIN/NUCLEIC ACID COMPLEXES	NUCLEIC ACIDS	CARBOHYDRATES	
X-RAY DIFFRACTION AND OTHER	11,630	556	580	14	12,780
NMR	1,918	73	383	4	2,378
THEORETICAL MODELING	288	19	23	0	330
TOTAL	13,836	648	986	18	15,488

Several new searching functions have been released. It is now possible to search by the number of chains on a structural backbone or in a complex. Users can also search by source organism, including synonyms and common names, so that searches on 'human' and 'Homo sapiens' return the same entries. The key word search function now performs both exact and partial word matching, and it is possible to query on the titles of entries. A new interface can reveal how many structures exist at some level in the Enzyme Commission (EC) hierarchy. This required the accurate assignment of enzyme

numbers to all relevant PDB structures and integration of EC nomenclature into the database system. Remediated files, related software, and update notices are archived at the Data Uniformity Project Web page at www.rcsb.org/pdb/uniformity/index.html. The home page has been revised to emphasize mirror sites, to permit both keyword and PDB ID searching, and to improve access to documents, format descriptions, and other materials.



CIFTr, a tool used by PDB staff in data processing that translates from mmCIF to PDB format, has been released publicly. The program works on UNIX platforms, and can be downloaded at <http://deposit.pdb.org/software/>.



The validation software used by ADIT to run checks on structures as a part of primary data processing and as part of data uniformity has been compiled into a suite of programs available for download. Designed to work with files in mmCIF or PDB format, the beta version of this validation software can be downloaded in binary form for SGI, SUN, and Linux platforms from <http://deposit.pdb.org/software/>. Reports produced include an Atlas entry, a summary report, and a collection of structural diagnostics including bond distance and angle comparisons, base morphology comparison (for nucleic acids), and molecular graphic images. In addition, reports from PROCHECK, NUCHECK, SFCHECK are also made available. The PDB has compiled a variety of structural genomics links at www.rcsb.org/pdb/strucgen.html

Taken from the PDB Annual Report

NOTICE

Crystallography beamlines on DIAMOND?

The planning for the design and building of the New DIAMOND synchrotron is well under way. Two bids from the Crystallography community have been submitted to the first stage. A proposed powder station will support the rapid collection of very high-resolution data suitable for structure solution and Rietveld refinement of inorganic and organic materials. A single crystal station has been designed to study the structures of molecules in their excited states, to probe *in situ* reactions, to carry out rapid and highly accurate charge density and anomalous dispersion studies, to investigate the relationship between molecular disorder and the physical properties of materials, and to develop mesomolecular crystallography. The powder bid is being coordinated by Jeremy Cockcroft (Birbeck College, London) (cockcroft@img.cryst.bbk.ac.uk) and the single crystal bid by Paul Raithby (U. of Bath) (p.r.raithby@bath.ac.uk). The first meeting of the DIAMOND Special Interest Group for crystallography will take place at the Nottingham BCA Spring Meeting.

Jeremy Cockcroft and Paul Raithby

The EPSRC Nat'l X-ray Crystallography Service is being expanded to enhance work with small and weakly diffracting crystals, to complement the existing services of handling twins and expedite, high-resolution studies. The service will benefit from coordinated use of advanced diffraction facilities of the Universities of Southampton and access to the Synchrotron Radiation Source (SRS) at Daresbury Laboratory, where Bill Clegg holds a formal Joint Appointment. The program will include user training, encouraged by EPSRC. Workshops and possible involvement in the experimental work. A call for applications will be issued, via heads of UK University chemistry departments. See www.soton.ac.uk/~xservice and www.ncl.ac.uk/xraycry for further details

Mike Hursthouse and Simon Coles, U. of Southampton

Bill Clegg, U. of Newcastle upon Tyne and Daresbury Laboratory

NOTICE

Silicates

The authors of the *Handbook of Mineralogy*, John W. Anthony, Richard A. Bideaux, Kenneth W. Bladh, and Monte C. Nichols have made available to the Mineralogy Soc. of America the full text of the 904 species published in Volume II (Silicates). Information about each silicate is contained in Adobe pdf files online. Try it out at www.minsocam.org/msa/handbook/handbook.lasso

NOTICE

ICDD resources



Awards. The Int'l Center for Diffraction Data (ICDD) received a generous donation from Howard McMurdie, Editor of Ceramics and Inorganics for the Powder Diffraction File (PDF) to establish a H. McMurdie Video Conferencing Center at the ICDD Headquarters. The Denver X-ray Conference Organizing Committee established the Jerome B. Cohen Student Award, to recognize outstanding achievements of student research in the field. Students interested in participating in the annual competition must submit papers, in final publication form, along with the required certification form (available at www.dxcicdd.com, or maguire@icdd.com).

The PDF The ICDD introduces the latest version of PDF-2, Release 2001 of the Powder Diffraction File, which contains 136,895 patterns with over 5,500 new additions. The file boasts over 87,500 experimental patterns in addition to over 49,000 patterns calculated from the ICSD (Inorganic Crystal Structure Database). Enhancements to ICDD's pricing structure include our new multiyear licensing policy.

PDF-4. The ICDD has also introduced a new product line, PDF-4. The PDF-4 databases are organized in a relational database format (RDB) with retrieval and viewing software integrated and bundled into a single product at low introductory prices. The ease of the RDB format provides the end user with numerous conveniences including query sorting capabilities for known physical properties, subfile designations, and search indexing. Additionally, an end user can perform 'on-the-fly' calculations to obtain fully digitized patterns which can be corrected for various experimental and instrumental factors and displayed using integrated viewing software (PCPDFWIN). Visit us on the Web at www.icdd.com.

NOTICE

ICSD For WWW

The Jan. 2001 version of the Inorganic Crystal Structure Databases ICSD-for-WWW contains several new features requested by users. The new features are described on <http://barns.ill.fr/dif/icsd/news.html> and may be tried on the ILL's server <http://barns.ill.fr/dif/icsd>. New features include: 1) Acrobat PDF output of calculated and indexed powder patterns (as an alternative to postscript) 2) Chime/PDB 3D-display of structures (as an alternative to VRML) 3) Username/Password access (as an alternative to IP names) see: <http://barns.ill.fr/dif/icsdpassword.html> 4) Various minor bug fixes. The present ICSD-for-WWW database from FIZ-Karlsruhe contains 57,195 entries. If you run down your own ICSD-for-WWW server, this version for SGI, Sun and HP server is available from: <ftp://ftp.ill.fr/pub/dif/icsd>.

ICSD User Group Newsletter 13

NOTICE

JobSpectrum.org

Seven months from its initial launch, JobSpectrum.org, the career website of the American Chemical Society is identified by CareerXroads 2002 as one of the top websites for jobs, resume and career management information. JobSpectrum is the total career resource web site for the chemical community and the place for chemistry-related career development resources.

The selection criteria included value of content, ease of access and navigation, real-world marketing strategy and technology, and business.

The top pharmaceutical companies and biotech firms listed by Hoover's have registered with JobSpectrum and used the service. Since inception, JobSpectrum has attracted 5,822 registered job seekers, over 1,000 registered companies, and resulted in over 12,000 applications, according to the data posted at its website, www.jobspectrum.org, as of February 19, 2002.

JobSpectrum is a joint venture of the ACS Publications and the ACS Membership Division.

NOTICE

SciDev.Net

A new independent website, SciDev.Net, will provide a forum for authoritative news, information and comment about how science and technology can help meet the needs of developing nations. The journals Nature and Science are providing free access to selected articles. Support and guidance is being given by the Third World Academy of Sciences, and funding is being provided by the UK Dept for Int'l Development, the Swedish Int'l Development Cooperation Agency and the Int'l Development Research Center in Canada. You can show your support by visiting the web site (www.scidev.net), registering your interest, and engaging in the debates.

NOTICE

Online Macromolecular Museum

The Online Macromolecular Museum (OMM) at www.clunet.edu is a site for the display and study of macromolecules. The OMM's exhibits are interactive tutorials on individual molecules with explanations of important biochemical features are linked to illustrative images of molecules. In order to view the macromolecular exhibits at the OMM you will need two, free items which you can access from the web site:

1. A FRAMES-capable browser. Netscape Navigator 4.73 strongly recommended but NOT Navigator 6 and NOT MS IE.
2. MDL Chemscape Chime (v.2.0+ recommended).

NOTICE

Geometry of crystals

www.polymorf.net/knowhere1.htm

Lesson on the geometry and symmetry of elements and minerals using Polymorf, a new math and science manipulative. The topological approach is used to characterize the structure of crystals in terms of linked polyhedra. Elements and minerals are classified according to their atomic packing and the percent occupation of interstitial voids. Numerous models built with Polymorf demonstrate the lattice structure, polyhedral framework, and crystal habit.

Rick Engel, morfun@polymorf.net

BOOK REVIEW

Books

The Basics of Crystallography and Diffraction - 2nd Edition, by Christopher Hammond, Publisher, Oxford University Press, May 2001, Hardback ISBN 0-19-850533-1, £49.95, Paperback ISBN 0-19-850552-3, £22.95.

Throughout, the text is very readable and the level of mathematics expertise is appropriate to the subject matter covered. Recommended for students and lecturers working in the area of crystallography and diffraction.

Reviews in Mineralogy and Geochemistry (RiMG) series. RiMG Volume 41 is titled *High Temperature and High Pressure Crystal Chemistry* and is edited by Robert M. Hazen and Robert T. Downs. Topics include the characterization, interpretation, and description of structural variations with temperature and pressure, and experimental techniques used to investigate them. It has a lenticular print on the front cover that is a short movie showing the structural change in quartz with changing pressure and temperature, there is a color signature, and a series of flip movies on the margins of chapter 4 showing structural changes. These and other animations can be found at www.geo.arizona.edu/zta/movies/crystal_movies.html. 596 pp. ISBN 0-939950-53-7. The cost is US\$27 for members and US\$36 for nonmembers.