

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President



Since I wrote the last letter for the *Newsletter* significant changes have occurred in my personal and professional life. After six years as Director of Research with responsibility for the Life Science program at the European Synchrotron Radiation Facility (ESRF) in Grenoble I have returned to my position at the University of Copenhagen as professor of structural chemistry. Formally this move implies that my IUCr nationality from 1 June has changed from French to Danish. The six years at the ESRF have been a very exciting experience, it has been great to work for one of the world's leading synchrotron facilities and be part of the management team that obtained the official approval to upgrade the ESRF. An extra benefit of living in France was the good insight I got into crystallographic life in France. I had the pleasure of participating in the annual meeting of the Association Française de Cristallographie (AFC) in July 2008 and could sample the broad crystallographic activities in France. As an example of the high level of activity of the AFC, I would like to praise their initiatives in bringing crystallography to the public. The AFC organized the large exhibition *Voyage dans le cristal* being held in Grenoble from April to September this year. I had the opportunity to visit the exhibit in May with Davide Viterbo, former member of the IUCr Executive Committee, and two new members of the Executive Committee, Elena Boldyreva and Louis Delbaere. This successful exhibition by the AFC could be an inspiration for other national crystallographic committees.

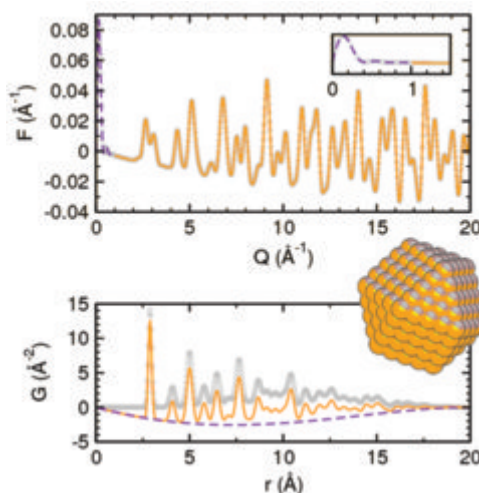
The increasingly important role played by large research infrastructures is one of the things that my appointment at the ESRF has made me very aware of. About 80% of the structures deposited in the Protein Data Bank have been determined using synchrotron radiation, justifying the statement that synchrotron radiation has revolutionized structural biology. New synchrotron facilities are under construction or are just becoming operational all over the world; this will have a great impact on a broad spectrum of the research represented by the IUCr. New exciting opportunities will be offered in the future by the free electron lasers (FEL), new brilliant X-ray sources with unique properties. X-rays and neutrons are complementary sources for the study of matter. Neutrons generated by the new powerful spallation sources will offer other new dimensions for crystallographic research. The links between crystallography and large research infrastructures generating X-rays and neutrons are already very strong, but likely to be even more enhanced in the future. As an example, the attendance of the annual Danish crystallography meetings almost doubled after they were organized jointly with the X-ray and neutron scattering communities, and very importantly the proportion of young scientists increased significantly.

I would like to conclude this letter by mentioning a problem that has become a major concern for me during the last six years. Large facilities are used more and more for crystallographic research and the scientists working there are responsible for providing the best service for the users that come to carry out their experiments. A prominent example concerns the beamlines for macromolecular crystallography. The scientists at the synchrotrons have invested enormous human resources into the automation of the beamlines making them so efficient that the users can control their experiments from their home laboratories. Many users take these well functioning beamlines for granted and often forget to recognize the efforts involved in creating the instrumentation, hardware and software. The lack of recognition from the users may have a negative effect on the beamline scientists that could eventually have a negative impact on beamline developments. It could be useful to have a dialogue between the communities of macromolecular crystallographers and scientists at the synchrotrons on this problem. Hopefully this could lead to the formulation of guidelines for an appropriate recognition of the use of large infrastructures.

Sine Larsen (slarsen@esrf.eu)

Relationship between the atomic pair distribution function and small-angle scattering: implications for modeling of nanoparticles

***Acta Cryst.* (2009). A65, 232-239 (doi.org/10.1107/S0108767309009714)**



Top: Simulated diffraction patterns from gold nanoparticles in the form of $F(Q) = Q[S(Q) - 1]$, the reduced structure function. The violet and gold lines indicate the small-angle and wide-angle scattering, respectively. Bottom: The resulting PDFs obtained by Fourier transforming the data in the top panel. Normally, nanoparticle PDFs are determined by excluding the SAS (gold), in which case they have a non-linear baseline that is characteristic of the nanoparticle's shape and size and can be reconstructed by measuring the SAS (purple).

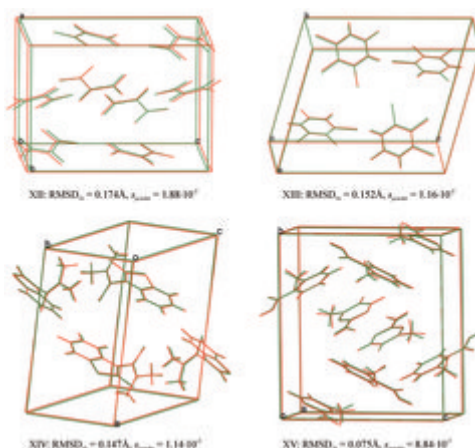
The atomic-pair distribution function (PDF) is emerging as a powerful tool for studying structure on the nanoscale. Small-angle scattering (SAS) also yields information about nanoscale density fluctuations in materials. This article presents a complete re-derivation of the PDF equations revealing the formal connection to the SAS equations and facilitating the combination of these methods. The SAS information is of particular value when modeling discrete nanoparticles as it yields the shape of the PDF baseline.

C.L. Farrow and S.J.L. Billinge

IUCR JOURNALS NEWS

Significant progress in predicting the crystal structures of small organic molecules - a report on the fourth blind test

***Acta Cryst.* (2009). B65, 107-125 (doi.org/10.1107/S0108768109004066)**



Overlays of the unit-cell contents of the observed crystal structures of the four blind test targets with one of the successful predictions for each. RMSD_{16} and s_{powder} are measures of the deviation between observed and predicted crystal structures.

Computational methods that have been developed for organic molecular crystal structure prediction have been tested in a fourth blind test, where 14 research groups attempted to predict the crystal structures of four targets, given only their chemical diagrams. The results demonstrate significant progress since previous blind tests; each crystal structure was correctly predicted by more than one participant and one group was successful for all four structures. Within the restrictions of the blind test, crystal structures of small rigid molecules seem to be predictable.

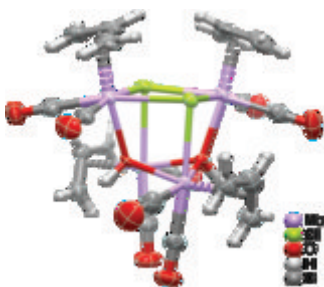
G. M. Day et al.

IUCR JOURNALS NEWS

Mo₄(η³-allyl)₄Cl₂(OH)₂(CO)₈: the first cubane-type Mo²⁺ organometallic complex with μ-OH and μ₃-Cl bridges

Mo₄(η³-allyl)₄Cl₂(OH)₂(CO)₈: the first cubane-type Mo²⁺ organometallic complex with μ-OH and μ₃-Cl bridges

Acta Cryst. (2009), C65, m168-m170 (doi.org/10.1107/S0108270109009512)



The tetrametallic Mo₄(η³-allyl)₄Cl₂(OH)₂(CO)₈ molecular unit.

An Mo²⁺ organometallic complex with a central trigonal prismatic [Mo₄(μ₃-Cl)₂(μ₃-OH)₂]⁴⁺ core, in which two of the faces are capped by μ₃-OH groups and the other two by μ₃-Cl anions, was synthesized and structurally characterized in the solid state. This complex constitutes the first example of an organometallic complex in which the central cubane core is composed of two distinct bridging moieties. The four crystallographically independent Mo²⁺ centres are further connected to allyl groups and CO molecules.

T.R. Amarante, I.S. Gonçalves and F.A. Almeida Paz

Combining crystallographic information and an aspherical-atom data bank in the evaluation of the electrostatic interaction energy in an enzyme-substrate complex: influenza neuraminidase inhibition

***Acta Cryst.* (2009). D65, 485–499 (doi.org/10.1107/S0907444909009433)**



Schematic of the active site of the influenza virus neuraminidase and its electrostatic interaction with different parts of the sialic acid inhibitor.

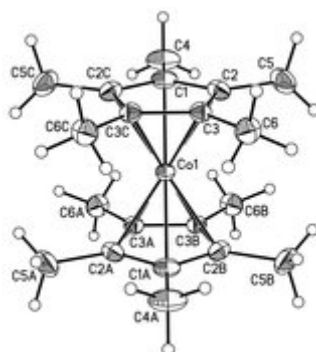
Since the electron density of a particular atom is determined by its surroundings, atomic electron densities are transferable to other sites with identical bonding environments. The University at Buffalo Databank of aspherical atomic densities is used to synthesize the electron densities of the influenza neuraminidase enzyme and 70 different inhibitors to evaluate the electrostatic enzyme-inhibitor interaction energy at an accuracy well beyond that of the point-charge approximation. Relative electrostatic interaction energies of the inhibitors and the effect of the Arg292→Lys mutation are calculated.

P.M. Dominiak, A. Volkov, A.P. Dominiak, K.N. Jarzembska and P. Coppens

Bis(η^5 -pentamethylcyclopentadienyl)cobalt(II)

Bis(η^5 -pentamethylcyclopentadienyl)cobalt(II)

Acta Cryst. (2009). E65, m391 (doi.org/10.1107/S1600536809007971)



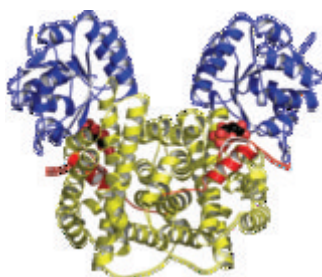
Decamethylcobaltocene (CoCp^*_2) is a widely used reducing agent that is of fundamental importance to the organometallic community, but surprisingly its crystal structure has not been reported in the literature. High-quality yellow-brown crystals were grown from a cold saturated solution in hexamethyldisiloxane, yielding a structure that is isomorphous with FeCp^*_2 and the low-temperature polymorph of MnCp^*_2 . The CoCp^*_2 molecule lies in a crystallographic $2/m$ position that is consistent with its inversion symmetry and staggered cyclopentadienyl rings.

M.M. Clark, W.W. Brennessel and P.L. Holland

IUCR JOURNALS NEWS

Geobacillus stearothermophilus 6-phosphogluconate dehydrogenase complexed with 6-phosphogluconate

Acta Cryst. (2009). F65, 450–454 (doi.org/10.1107/S1744309109012767)



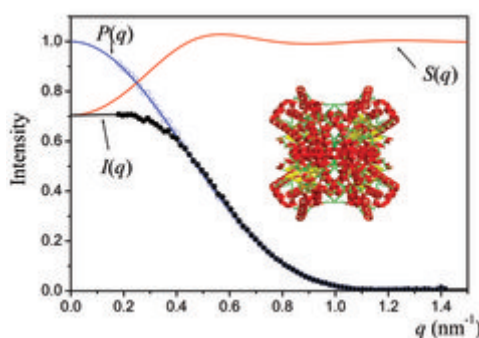
Secondary and domain structure of the Gs6PGDH dimer. The N-terminal domains are blue, the central domains yellow, the C-terminal domains red. The ligand 6PG is shown as van der Waals spheres coloured C black, O red and P orange.

The structure of *Geobacillus stearothermophilus* 6-phosphogluconate dehydrogenase (Gs6PGDH) complexed with 6-phosphogluconate is reported. 6PGDH is a highly conserved enzyme with conservation most pronounced in the N- and C-terminal domains, which contribute to the active site, compared with the central domain, which is involved in dimerization. 6PGDH is a potential drug target for the parasite *Trypanosoma brucei*, which causes African sleeping sickness. The *T. brucei* enzyme is unsuited for ligand studies but the straightforward crystallization means that Gs6PGDH provides a surrogate model for inhibitor design.

S. Cameron, V.P. Martini, J. Iulek and W.N. Hunter

High-pressure small-angle neutron scattering studies of glucose isomerase conformation in solution

J. Appl. Cryst. (2009). 42, 461-468 (doi.org/10.1107/S0021889809007456)

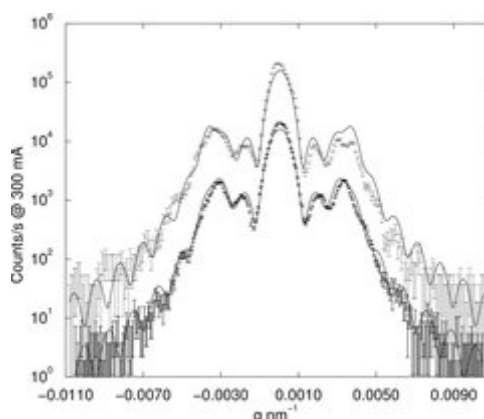


The glucose/xylose isomerase from *Streptomyces rubiginosus* was studied by means of small-angle neutron scattering (SANS) in the pressure range 0.1–150 MPa. Since this relatively large (172 kDa), almost spherical protein is not sensitive to pressure and temperature changes in a broad range, it was selected as a very good candidate for a secondary standard in SANS experiments. Correction of the intensity $I(q)$ resulting from intermolecular interaction described by the structure factor $S(q)$ is also discussed.

E. Banachowicz, M. Kozak, A. Patkowski, G. Meier and J. Kohlbrecher

Development of new apertures for coherent X-ray experiments

J. Synchrotron Rad. (2009). **16**, 358–367 (doi.org/10.1107/S0909049509003720)



Fraunhofer diffraction patterns in the horizontal (bottom) and vertical direction (top, multiplied by 10) of a 6 mm x 6 mm novel GaAs aperture generated with partially coherent 3.1 keV X-rays. The solid lines are least-squares fit of the model presented. Note that refraction effects cause the second order fringes to be more intense than the first order ones.

In a coherent X-ray scattering experiment at synchrotron sources, the incident beam must be spatially filtered by slits on a length scale smaller than the transverse coherence length of the source (10–100 μm). The Fraunhofer diffraction pattern of the slit is an important source of background in these experiments. This paper shows how one might reduce the diffracted intensity in the tail of the diffraction pattern by making slit edges softened by partial X-ray transmission using a method in visible optics called apodization.

E.M. Dufresne, S.B. Dierker, Z. Yin and L. Berman

MEETING REPORT

Zürich School of Crystallography. Bring Your Own Crystals

Zürich, Switzerland, June-July, 2008

The second Zürich School of Crystallography was intended for Masters and Ph.D. students, and postdocs in the molecular and solid-state sciences, who do not have access to crystallographic courses at their own institution. The twenty participants (12 women and 8 men) came from Croatia, Finland, France, Germany, Italy, Poland, Portugal, Slovenia, Switzerland and Turkey. The personal impressions of one of the students are given below.

Tony Linden, Hans-Beat Bürgi, School Directors

The Zürich School of Crystallography 2008 - The Meaning Behind the Numbers: A Student's Perspective



For me crystallography is a tool for the investigation of the conformational and host-guest properties of my compounds, as well as an analytical method, alongside NMR and mass spectroscopy, for the confirmation of the structure of my synthesis product. However, determining a crystal structure requires training and knowledge before it can be done reliably. I had some experience in solving crystal structures, but wasn't able to make the connection between routinely done procedures and theory, which was the reason for attending the Zurich School of Crystallography. The course covered growing single crystals, collecting and processing data, solving and validating the structure and reporting the results. The theoretical information seemed overwhelming but during the practical sessions, it was easier to see where the theory came into play. I was extremely grateful to have the help of the tutors when I was puzzled about something. The small size of the group made the learning environment intimate and it was possible to get to know everyone involved. It was great to meet people from different areas (and countries) and I especially enjoyed the discussions at the end of the day. Before attending the school, I used to check crystallographic parameters without understanding the meaning behind the numbers. Now I feel more confident in evaluating my crystal structure solutions. In every respect, I was very pleased with the school and gained more than I had anticipated.

Kirsi Salorinne

MEETING REPORT

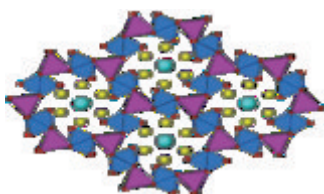
IUCr Congress and General Assembly



Osaka, Japan, August 2008 www.crsj.jp/iucr2008/

This is a continuation of the reports on the XXI Congress that can be found in Volume 16, No. 3 & 4

Crystallochemical Basis of Synthetic Mineral Immobilisation (KN11)



Tim White (MSE-NTU, Singapore) reviewed methods for immobilising pollutants by crystal chemical and mineralogical principles. Spent nuclear fuel, slag heaps, incinerator ash and tailing dams are major sources of inorganic waste. Key principles for immobilization in a mineral matrix are: (1) toxic metals should be incorporated in their least toxic chemical states (for example, As^{5+} and Cr^{3+} instead of As^{3+} and Cr^{6+}); (2) crystal structures are preferred that have multiple cation and/or anion acceptor sites as this minimizes the number of phases required; (3) phases with large numbers of appropriate cation acceptor sites are advantageous, as they result in higher waste loadings and less 'bulking' of the waste product. The crystallochemical bases (e.g., framework distortion, polysomatism and incommensurate phases) of synthetic mineral immobilization have been described for several structure-types among which: perovskite, pyrochlore, zirconolite, hollandite and apatite. In particular, the flexibility of the structure of apatite in accepting a variety of ions, via different mechanisms, has been discussed in detail on the basis of several results obtained in the laboratory of the lecturer.

Giovanni Ferraris

Advances in Grazing Incidence, Reflectivity and Diffuse Scattering (MS2)

Sponsored by the IUCr Commission on Small-angle Scattering, this symposium focused on 'Advances in grazing incidence, reflectivity and diffuse scattering'. It encompassed current developments across the range of scattering in a reflection geometry, especially X-ray and neutron reflectivity (XR and NR), and grazing-incidence small-angle X-ray and neutron scattering (GISAXS and GISANS), and brought together several leading international experts.

P. Müller-Buschbaum (Germany) spoke on 'Recent developments in GISAXS and GISANS - nanobeams and *in situ* kinetic investigations'. He described how it is possible at the 3rd generation X-ray synchrotrons to combine microbeams and nanobeams in grazing incidence geometry to tune surface sensitivity, and thus to distinguish surface from volume structures during *in situ* kinetic studies of thin films. The potential of the method was illustrated by *in situ* GISAXS studies of nanoparticle Au sputtering on polymer fibers, a critical technology for developing next-generation photovoltaics.

T. Matsushita (Japan) spoke on 'Quick X-ray reflectometry in simultaneous multi-wavelength dispersive mode'. He described how curved crystal optics, used to provide fast time resolution in energy dispersive X-ray absorption spectroscopy, could be applied in energy-dispersive XR studies to improve the time

resolution from minutes or hours in 'conventional' XR to millisecond time resolution in energy-dispersive XR. The method was illustrated with reflectivity studies of 20 ms time resolution for a rotating specimen comprising a 14.3 nm Au nanolayer film on a Si substrate.

Returning to GISAXS fundamentals, B. Lee (USA) spoke on 'Structural characterization using the multiple scattering effects in GISAXS'. Whereas the distorted wave Born approximation has been successful in describing GISAXS data, multiple scattering can complicate the picture. Its analysis can be simplified by using interference effects between scattering from the incident and from the reflected X-ray beams in incident-angle-resolved GISAXS (IAR-GISAXS). By illustration, Lee described studies of virus particles in polymer films on Si substrates.

The unique advantages provided by the neutron scattering isotope effect were highlighted by A. Takahara (Japan) in his talk, 'Neutron reflectivity study of chain conformation in polyelectrolyte brushes at the liquid interface'. His account of an NR study of polymer brushes on quartz substrates immersed in water demonstrated the power of D_2O/H_2O neutron contrast variation studies to tune the film density profile as a function of swelling and processing. Takahara showed how hydrophobic and hydrophilic interfaces can be distinguished, and the effects of the aqueous phase ionic strength on the conformation and surface properties of the brushes determined. The brushes can be manipulated by exploiting their mutual adhesive properties using microfluidic principles.

A combination of GISAXS and grazing-incidence X-ray diffraction (GIXD) methods to characterize, *in situ*, the vacuum growth and catalytic reactivity of nanoparticles on an oxide surface was described by R. Lazzari (France) who spoke on 'Following growth and catalytic reaction of oxide supported metal nanoparticles with GISAXS'. Using a high-vacuum chamber to give low background, these methods permit experimental testing of GISAXS data modeling and simulations. The growth laws and thermodynamics for Au nanoparticles on TiO_2 were established, revealing a striking self-similar behavior.

The symposium retained an audience of 60 to 80 persons throughout, and clearly demonstrated the importance of such measurements in the development of advanced materials critical to emerging nanotechnologies.

Andrew Allen and Moonhor Ree

MEETING REPORT

11th Heart of Europe bio-Crystallography Meeting



11th Heart of Europe bio-Crystallography Meeting

Greifswald, Germany, September 2008

www.chemie.uni-greifswald.de/~biochem/hec-index.html



Participants of HEC-XI in Greifswald, Germany.

The Heart of Europe bio-Crystallography Meeting entered its second decade on September 25, 2008. The meeting was organized by the Molecular Structural Biology Group of Ernst-Moritz-Arndt U. of Greifswald. The meeting attracted 113 participants from bio-crystallography groups in Germany, Poland, and the Czech Republic. During the three days of the meeting, 35 lectures were presented mostly by students and young scientists. The keynote HEC Lecture was given by Poul Nissen (University of Aarhus) on the crystal structure of the sodium-potassium pump. The HEC Prize for the best lecture was awarded to Linda Schuldts (EMBL Hamburg Outstation) for her talk entitled: Three-dimensional crystal structure of DapD from *M. tuberculosis*. The prize was a copy of the *International Tables for Crystallography*, Vol. A, which was generously sponsored by the IUCr.

Social activities included two informal evening get-togethers and a boat ride on the Baltic Sea.

A publication entitled *10 Years of Heart of Europe bio-Crystallography Meetings*, edited by Mariusz Jaskolski and Michal M. Sikorski (Inst. of Bioorganic Chemistry of the Polish Academy of Sciences, Poznan, Poland), was unveiled. This book summarizes information about all previous meetings including posters, programs, reminiscences of organizers and numerous photographs and documents how well the HEC community has flourished over the last decade.

The next HEC meeting, scheduled for September 24-26, 2009 will be organized by Pavlina Rezacova and her group in Trest, Czech Republic (www.img.cas.cz/hec).

Pavlina Rezacova

MEETING REPORT

1st SESAME-JSPS school on Synchrotron Sciences



1st SESAME-JSPS school on Synchrotron Sciences

Cairo, Egypt, November 2008 <http://www.sesame.asrt.sci.eg/>

SESAME, the Synchrotron light for Experimental Science and its Applications in the Middle East (www.sesame.org.jo) is a synchrotron facility being built in Jordan under the auspices of UNESCO. Full members of the project include Bahrain, Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, the Palestinian Authority and Turkey. Moreover, France, Germany, Greece, Italy, Japan, Kuwait, the Russian Federation, Sweden, the United Arab Emirates, the UK and USA will act as observers. The Japanese Society for the Promotion of Science (JSPS), Japan's leading funding agency has implemented far-reaching programs to fund domestic and international scientific projects for 70 years.



The first SESAME-JSPS school on synchrotron sciences was held Cairo U. About 20 Japanese scientists offered lectures and hands-on practical sessions covering a wide range of synchrotron related fields; from archeology to structural biology and from electronic structure to materials science.



The co-chairs of the school, Tarek Hussein (President of the Egyptian Academy of Science) and Osamu Shimomura (Director of the Inst. of Material Science, KEK, Japan), welcomed the attendees and Herwig Schopper (former President of the SESAME council) described the status and future prospects for SESAME. Kaouro Ishikawa (Japanese ambassador to Egypt) emphasized Japan's commitment to promoting and supporting science and technology in the region and Hany Helal (Egyptian Minister of Higher Education and Scientific Research) emphasized his country's determination to support SESAME. This session was followed by presentations by Wolfgang Eberhardt (Director of BESSY, Germany), Paul Dumas (SOLEIL, France), Amor Nadji (technical director of SESAME), Jun Akimitsu (Aoyama-Gakuin U.),

and Osamou Shimomura (KEK). A banquet was served aboard a cruise ship on the Nile with traditional Egyptian food, music and dance.



Salwa Sabet (center) prepares the wet lab for protein crystallography.

Topics covered included the storage rings (S. Tantwai, SSRL and S.Kurokawa, KEK), applications in structural biology (M. Yousef, KEK/Cairo U., N. Igarashi, KEK, and M. Yamamoto, RIKEN/Spring8), basics of crystallography (H. Sawa, Nagoya U.), nanotechnological applications (M. Sakata, Nagoya U.), powder diffraction/material science (K. Kato, RIKEN/Spring8 and P. Scardi, ELETTRA, Trieste), electronic structure (A. Kimura, Hiroshima U), photo emission spectroscopy (H. Kumigashira, Tokyo U.), X-ray imaging (A. Momose, Tokyo U.) structural dynamics (S.Adachi, KEK), and applications in archeology XAFS (K. Asakura, Hokaido U., I. Nakai, Tokyo U., and M. Pantos, Daresbury).



Osamu Shimomura introduces SR facilities in Japan.

Each scientific session was followed by 'meet the expert' discussions where scientists from the SESAME countries were given the opportunity to consult one-to-one with leading experts regarding experimental designs and potential collaborations. About 200 students and scientists from almost every SESAME country attended the school.

Hands-on data analysis laboratories were run during the last two days of the school. Students from Algeria, China, Egypt, India, Iran, Italy, Jordan, Morocco, Pakistan, USA and Yemen, participated in the practical sessions which covered structural biology, electronic structure, archeology, material science and XAFS. The practical sessions were led primarily by the Japanese scientists, assisted by Egyptian faculty members. Cairo U. provided the lecture halls, wet labs and computational facilities for the practical sessions. At the closing session, the students presented their projects to the audience.



Japanese scientists enjoying traditional Egyptian food.

Delegates from SOKENDAI (the graduate university for advanced studies in Japan) Misa Miyai and Masani Gomita gave talks about graduate study opportunities in Japan. The SESAME-JSPS school was sponsored and supported by the Academy of Scientific Research and Technology of Egypt, DAAD (Germany), the Italian and French embassies in Cairo, and ICTP (Trieste, Italy). Exhibitors included Oxford diffraction and PanAnalytical. The success of the 1st SESAME-JSPS school was really astonishing and Shimomura (KEK) is already discussing with SESAME directors the location and plans for the next school.

Mohammad Yousef, Tarek Hussein and Osamo Shimomura

MEETING REPORT

38th National Seminar on Crystallography



38th National Seminar on Crystallography



Mysore City, India, February 2009 <http://38nsc2009.synthasite.com>



Left to right: B. Basvalingu, J.K. Dattagupta, G.R. Desiraju, K. Lal, V.G Talwar, R. Chidambaram, S. Banerjee, M. Vijayan, K. Byrappa and R. Somashekar at 38th NSC in Mysore, India.

The conference was held February 11-13, in Mysore City, which has the reputation for architectural heritage and colorful streets. The conference was opened by R. Chidambaram, former IUCr Vice-President and current Principal Secretary to the Government of India. A total of 350 delegates included people from the US, the UK, Germany, France, Italy and Japan. The conference was organized into two parallel sessions covering several topics including crystal engineering, drug receptor and antigen-antibody recognition, diffraction methods, charge density, computational crystallographic database research, powder X-ray diffraction, inorganic and mineral structures, teaching methods, layers, thin films and polymers. A total of 201 posters were displayed. The local committee organized a special cultural program along with a conference dinner. The lecture by M. Vijayan on 'Form and functions in proteins' was attended not only by the official delegates but by scores of students from nearby colleges and research institutes. The program concluded by honoring senior teachers of the U. of Mysore at an evening function. Financial support by MARresearch, Rigaku, PANalytical and others are greatly appreciated.

K. Byrappa and R. Somashekar

REGIONAL NEWS

The ECA Executive Committee's 'Winter Meeting' 2009

The Executive Committee of the European Crystallographic Association (ECA-EC) winter meeting was held February 27 – March 1, in Budapest, Hungary. Sine Larsen took part in her unique situation as both the President of IUCr and Vice-President of ECA.



The Participants of the 'Winter Meeting' of the Executive Committee of the ECA, held in February 2009 in Budapest, Hungary at the 'Presidential Dinner'. From left to right: Süheyla Özbey (ECM25), Engin Kendi (ECM25), Engin Ozdas (ECM25), Luc van Meervelt (Officer), Jordi Rius (EPDIC), Sine Larsen (IUCr President, ECA Vice-President), John R. Helliwell (President), Petra Bombicz (Secretary), Santiago Garcia-Granda (Officer), Chris Gilmore (IUCr representative), Hartmut Fuess (Past-President, ECM26), Radomír Kuzel (Treasurer), Andreas Roodt (Officer) and Massimo Nespolo (Education Coordinator and Webmaster). The ECA President, John Helliwell, opened the meeting by summarising ECA strategy and covering the numerous matters arising from the minutes of the ECA-EC 2008 meetings held in Budapest and Osaka. One highlight covered was the work of the ECA and its regions, namely the activities of the newly founded Union of the Regional Committee of Crystallographers from Algeria, Latvia, Morocco, Tunisia, Turkey and Ukraine and a report received from Engin Kendi, Vice-Chair of the group. Another highlight was the discussion on establishing a 'General Interest Group Network of Young Chemists' in the ECA region. The nucleating centres would be the existing British and Spanish unions of young crystallographers. Such a GIG (General Interest Group) would widen the scope covered by existing ECA SIGs. There is also an increased focus on the education of future generations of crystallographers at all levels. One major aim is the establishment of a European Graduate School of Crystallography (Masters and PhD) as soon as possible with the EC's ERASMUS MUNDUS being one candidate scheme to seek funding; this effort is being spearheaded by Massimo Nespolo.

Chris Gilmore, as IUCr delegate to the Committee gave an overview of a variety of matters including the deepening link between the International Union and the ECA, one of its Regional Associates, and of the current big push by the IUCr to update the World Directory of Crystallographers which will relate well to the ECA's work to increase the number of its individual members. Sine Larsen reported that the transformation of *Acta Crystallographica E* to an open access journal has been successful as measured by the still very large number of submissions and the better balance of income and expenditure. John Helliwell is willing to coordinate input, via this Newsletter or by direct contact, for any colleagues within Europe that might be experiencing difficulties with the new *Acta Cryst E* arrangements. Through the work of the Treasurer, Radomír Kuzel, the number of ECA Corporate Affiliate Members (CAMs) has nearly doubled in the last year. Radomír is also making a continuous effort to increase the number of individual members of the ECA. Luc van Meervelt led the discussion on evaluating the bursary funding applications from the organizers of 2009 ECA Schools/Conferences/Workshops. This led to some very difficult decisions and the

general conclusion that applicants should be sure to respect the blackout periods around ECMs or IUCr Congresses (it should be noted that in a Congress year ECA still funds bursary applications). The next application deadline is in August 2009 for 2010. Santiago Garcia-Granda led the discussion on the ECA SIGs and presented an updated table of performance metrics, i.e. an evidence-based-system for monitoring of the performance of the SIGs, which aims, as efficiently as possible, to increase their performance. A few SIGs also have newly elected Conductors. Massimo Nespolo suggested taking into account their responsiveness to the EC call for microsymposia and keynote lectures for the forthcoming ECMs. Finally, the renewed focus area concept was reviewed and found to work well, for example for ECM25 programme planning; liaison between SIGs was actively encouraged and worked quite well.

The year 2009 is an election year for the ECA, i.e. new officers and members of the EC will be elected. Nominations are welcome following Statute 10 (<http://www.ecanews.org/statute.php>):- 10.3 The Council appoints the members of the Executive Committee on the proposal of the Committee or of at least five (5) Councillors.. The current EC, as per this statute reached a consensus on a set of recommendations that will be presented to the ECA Council. The ECA-EC auditors will also be nominated forthwith for approval by the ECA Council. The need of having at least one representative from each focus area on the EC was emphasized.

The ECA Perutz and Bertaut Prizes Selection Committees work independently from the ECA-EC and were respectively chaired by Andreas Roodt and Santiago Garcia-Granda. The results are now announced and are: Lynn McCusker is the recipient of the Max Perutz Prize and Lukas Palatinus is the recipient of the Bertaut Prize.

The next (ECM25) and future ECMs (ECM26 and ECM27) organisers, respectively, Engin Kendi (with Suheylyla Ozbey and Engin Ozdas), Hartmut Fuess and Karl Tornroos, presented their organisation progress. In Istanbul (ECM25) this year, the 25th anniversary of the European Crystallographic Meetings and the first discussions of forming an ECA, will be celebrated with a special event. At ECM26 a special feature will be joint symposia with the EPDIC and thus promises a relatively larger meeting and exhibition; Jordi Ruis, President of EPDIC, was present at this committee meeting, and also reported. ECM27, being held in 2012, will obviously highlight the 'Friedrich, Knipping and von Laue experiment centennial'. The bids from Greece (Athens) and the UK (Warwick) to host ECM28 to be held in 2013 will be examined at the ECA Council Meetings to be held within ECM25.

The ECA-EC hopes to meet you at ECM25 in Istanbul, Turkey, August 16-21, 2009.

For information on the European Crystallographic Association please visit the ECANews website: www.ecanews.org.

REGIONAL NEWS

Associazione Italiana di Cristallografia (AIC)



The new AIC Council at its first meeting in Milano. Seated left to right: Roberta Oberti, Carlo Mealli, Norberto Masciocchi. Standing left to right: Valeria Ferretti, Paola Bonazzi, Piero Macchi, Giuseppe Zanolli, Alessia Bacchi, and Lucio Zanolli.

In January 2009, the newly elected board of the AIC took office. The President Carlo Mealli (chair of the XX IUCr congress, Florence 2005) and eight councillors, including the past-president Roberta Oberti, will be in charge until 2011.

The success of the XX IUCr congress has had a significant impact on the Italian crystallographic community, producing great enthusiasm for new initiatives. Schools, workshops and meetings are now organized in a broader international framework. In 2007, the Italian National Congress became the first meeting of the Italian and Spanish Crystallographic Associations (MISCA). The event was preceded by a jointly organised school on protein crystallography and the second MISCA is scheduled in Spain next year. Among other initiatives in 2006, an IUCr school in basic crystallography was held in Pontignano Tuscany, and an AIC school on polycrystalline materials was organized in Martinafranca (near Bari). In this place, also a school on charge density. Another AIC school on polycrystalline materials was held in cooperation with the Swiss Crystallographic Assn. at the Paul Scherrer Inst. in Villigen (CH) and it will become a regular biennial event. This year, reviving a 30-year-old tradition, a school on scattering techniques featuring an international teaching staff will be held at the U. of Camerino (August 30-September 4, 2009: <http://web.unipmn.it/~chimfis/AICS2009/>). A thriving AIC subgroup on crystal growth is planning an international school on 'Adsorption, Absorption and Crystal Growth' in Gargnano near Brescia in 2010. International workshops on crystallographic methods are regularly organized in Bari by Carmelo Giacobazzo and his group. The most recent, PHARE 2009, attracted 90 participants. But the jewel in the crown of international crystallographic education remains the Erice schools that have been organized by Lodovico Riva and Paola Spadon for the past 35 years.



The gold medal 'Mario Mammi'

To celebrate the 40th anniversary of the association in 2007, a gold medal was coined to honor the memory of the former president and founder, Mario Mammi. The Mammi prize will be awarded every

other year to a leading scientist under the age of 60, who has achieved outstanding results in the field of crystallography while working in Italy. The recipient of the first 'Mammi' medal was Giuseppe Zanotti (U. of Padova) for contributions in bio-crystallography. This year, an international jury has just awarded the prize to Giovanni Luca Cascarano (CNR-IC, Bari) for his seminal contribution to the design of new methodologies for the solution of the structures of biological macromolecules.



Near Salerno, venue of the AIC national congress (September, 2009)

Other AIC prizes are the Mario Nardelli medal (former president of both the AIC and IUCr), that is annually awarded to a crystallographer under 36 years of age, and a diploma for the best university thesis in crystallography. This year's winners are Nicola Casati and Illio Miccoli, respectively, and all the prizes will be awarded during the AIC Congress in Salerno (September 20-23, 2009; www.cirpeb.unina.it/aic2009/intro.html), that is jointly organized by the Universities of Salerno and Napoli with a special focus on the crystallography of polymers. Pioneering work in the field was carried out in this region by Paolo Corradini. All the classical topics of crystallography will be covered. The Italian community is proud to announce that IUCr president Sine Larsen is among the invited speakers

Finally, in September 2011, the Italian National Council of Research (CNR) will host the General Assembly of the International Council of Science (ICSU) that joins 27 Scientific Unions. In conjunction with this meeting, the AIC has been asked to organize a one-day scientific symposium. Topics of social interest (health, environment, innovative materials and more) shall be discussed by renowned speakers, including Nobel laureates. The fundamental role played by crystallography in modern science and the active presence of the IUCr within ICSU will be highlighted.

Details (in Italian and English) of all AIC activities including the history and programs of the Association and individual members can be found at the new website (www.cristallografia.org).

Carlo Mealli

OBITUARY

Hans C. Freeman (1929-2008)

Hans Freeman, Emeritus Professor at the U. of Sydney, died on November 9, 2008. He authored over 160 research papers and received practically every honor available to a chemist in Australia including the Burrows and Leighton medals of the Royal Australian Chemical Inst. and the Craig medal for chemistry from the Australian Academy of Science. He was elected as a Fellow of the Academy in 1984 and was recognized by the Australian Government for contributions to chemistry by being made a Member of the Order of Australia in 2005. Hans excelled in teaching, research, and service to the community. His pioneering research achievement was to establish the field of protein crystallography in Australia and to lead the team that solved the first structure of a 'blue' copper protein, plastocyanin. He was in the laboratory until a few weeks before his passing doing what he loved best. He will be sadly missed by all who had the privilege to know him.

Hans was born in Breslau, Germany in 1929, his family left for Australia in 1938. He received an MSc (1952) and PhD (1957) from the U. of Sydney. He was awarded a Rotary Foundation Fellowship (1952-3) to spend time at the California Inst. of Technology where he learned the fundamentals of crystallography with Eddy Hughes. From the outset, his interest was in molecules of biological significance. The structure of biuret hydrate formed the basis of his PhD dissertation. From there he refined the focus of his work to metal complexes of peptides, and then later to metalloproteins.

In 1970 the U. of Sydney offered Hans an opportunity to explore new areas of research and the first protein crystallography laboratory in Australia was formed. He dedicated the first goal of the laboratory

to the solution of the structure of plastocyanin. The visualization of the structural basis for the 'blueness' of 'blue' copper proteins was a significant achievement in the field of bioinorganic chemistry.

Hans was instrumental in the formation of the Society of Crystallographers in Australia (SCA, later to become SCANZ) and was elected its first president in 1976. He was the program Chair for the very successful 1987 IUCr Congress in Perth and the residual income from the Congress has been used to fund travel by Australian and New Zealand students and to bring a distinguished lecturer to local meetings.

Hans was a charismatic lecturer for whom teaching was a love and a privilege and never an obligation. He continued teaching a special first year class long after his formal retirement. He was conscious of the fact that Australia suffered from a tyranny of distance that meant senior students had fewer opportunities than those in the northern hemisphere to interact with leading researchers. In 1972, he was instrumental in the formation of the Foundation for Inorganic Chemistry at the U. of Sydney, that each year since has brought one or two international scientists to the school to deliver a series of lectures.

Hans co-authored a report for the Australian Academy of Science entitled 'Small Country, Big Science' highlighting the need for Australian scientists to have access to major research facilities such as high-energy nuclear facilities and synchrotron sources. As a result of the report, the government funded Australian scientists to travel to overseas facilities and established the Australian Synchrotron Research Programme of which Hans was a board member until its incorporation into the Australian Synchrotron earlier this year.

Hans leaves behind a legacy of significant research, institutional innovations and generations of students imbued with a love of science.

Mitchell Guss

OBITUARY

John Robert (Bob) Carruthers (1945-2009)



Bob graduated from St. Edmund Hall (Oxford) having completed his Part II year doing copper chemistry with Francis Rossotti. He worked for his D. Phil. with Keith Prout and Francis, and became interested in crystallography. For one of the materials he worked on, he observed 'When the diffraction pattern was indexed, it became apparent that the crystals were unlikely to be orthorhombic, as a strange set of absences were found'. The crystals were twinned, 'overlapped reflections were arbitrarily assigned half the measured intensity until a program was written which would include both components in the least squares'. 'As there was not sufficient memory, it was necessary to rewrite the program in machine language'. Machine languages are basic to the electronics of the computer, and the programmer has the power and the responsibility of working hands-on with every memory location. So began Bob's life with computers, and his exceedingly productive partnership with John Rollett.

In 1969, Bob was awarded a fellowship from the Accademia Nazionale dei Lincei and the Royal Society, allowing him to work in Rome with Riccardo Spagna re-implementing the Rollett AUTOCODES symbolic language in FORTRAN. This program included features such as rigid-body constraints and some of the underlying data-structure can still be found in CAOS (Cerrini S. & Spagna R. 1977) crystallographic software for a mini computer.

Returning to Oxford, he worked with Rollet and Prout, re-writing the program from scratch. This new program, CRYSTALS, could handle up to 9 twinned components and had a good range of restraints (including facilities now often called SIMU and DELU). Perhaps the most novel feature was 'user-defined restraints', in which users could define their own equation of restraint as part of the input data, which was then analytically differentiated by CRYSTALS. The equation parser and differentiating engine were all written in beautiful FORTRAN and are still working, largely unmodified, in the current version of CRYSTALS. Bob's attitude toward programming combined a meticulous attention to detail with a far-reaching ability to plan on an expansive scale.

After his Postdoc, Bob started writing data-archiving software for Oxford U. Computing Service. However, he continued to work on CRYSTALS whenever he could and completely re-wrote the underlying data management for a third time when the university upgraded its mainframe to an International Computers Limited (ICL) 2980.

Around 1979, Bob went to work for Control Data Corporation, implementing meteorology programs on supercomputers. He spent most of his career implementing very large FORTRAN program systems and in recent years modernizing massive legacy packages. Weather forecasting profited from his work, but there is no doubt that crystallography lost an outstanding programmer.

When not working with computers, Bob was a dependable drinking companion and a formidable bar billiards enthusiast. Some of us still remember Bob and George Sheldrick, with other young crystallographers, trying to drink the bar dry at ECM 4 in Oxford in 1977. His brilliance as a scientist did not spoil his personality - he was always modest, amiable and good fun.

David Watkin

AWARDS AND PRIZES

Colman Wins Major Science Prize



Peter Colman (Photo courtesy of Samar Hasnain)

The \$50,000 Victoria Prize, one of Australia's most prestigious science prizes, has been awarded to eminent biomolecular scientist and long-term synchrotron user Peter Colman.

Peter Colman, Vice-President of the IUCr, is head of structural biology at the Walter and Eliza Hall Inst. in Melbourne. He received the Victoria Prize for his pioneering contribution to the development of Relenza(TM), the world's first neuraminidase inhibitor to treat the influenza virus.

In the late 1980s, Peter (then at CSIRO) worked with Graeme Laver (Australian National U.) and Jose Varghese (CSIRO) to create high-resolution images of the atomic structures of the molecules that control the way the flu virus spreads and infects neighbouring cells. Neuraminidase is an enzyme on the surface of the flu virus that enables the virus to enter and infect new cells. Relenza blocks the action of the neuraminidase enzyme in a way that works with all known strains of the flu virus.

AWARDS AND PRIZES

Ludo Frevel Scholarships



www.icdd.com

The ICDD Ludo Frevel Crystallography Scholarship Committee has selected ten recipients for the 2009 Scholarship Program. These recipients were selected, on a competitive basis, from forty-five commendable applications received by the ICDD Scholarship Committee. The recipients are: **Tobias Beck**, Goettingen U., Germany (Metal Sites in Proteins), **Hui Li**, Chinese Acad. of Sciences, P.R. China (GaN and AlN Based Diluted Magnetic Semiconductor and Superconductor, and eight in the USA, **Olaf Borkiewicz**, Miami U., (Actinide Sequestration in Low Temperature Growth of Apatite), **Dejan-Kresimir Bucar**, U. Iowa, (Metallosupramolecular Capsules with Nanometer-Sized Cavities Solid State), **Amado Guloy**, Northwestern U. (Charge Density Wave), **E-Wen Huang**, U. Tennessee (Mechanical Behavior of a Nano-particle Strengthened Nickel-based Alloy), **Andrey Ivankin**, Illinois Inst. Tech. (Determining the Role of Cholesterol in Cell Membrane Physicochemical Properties: and Insight from Synchrotron X-ray Scattering), **Christian Long**, U. of Maryland (Structural Phases in Combinatorial Thin-Film Libraries Using Non-Negative Matrix Factorization), **Mary Louie**, California Inst. of Technology (Phase Transformation Hysteresis), **Anna-Gay Nelson**, Auburn U. (Structural Chemistry of Actinide Shoshonites for Storing Radionuclides).

Each student will receive \$2,500 to assist in the continuation of studies in his or her selected field of crystallographic research.

These scholarships are made possible through corporate and private donations. If you would like information on how you can make a tax-deductible donation please contact the ICDD.

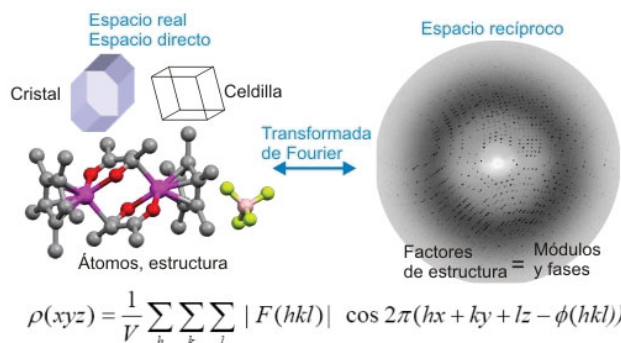
NOTICE

New Crystallography Website

www.xtal.iqf.csic.es/Cristalografia/

9. Cálculo en Cristalografía

Si a la izquierda de la pantalla no se muestra el menú de estos apuntes, [use este enlace](#).



El lector que haya llegado hasta este capítulo de un modo secuencial, se habrá dado cuenta de que, al margen del **problema de la fase**, la relación entre el experimento de difracción (espacio recíproco) y la estructura de un cristal (espacio directo) está mediada por una función del tipo transformada de Fourier, que es la densidad electrónica: $\rho(xyz)$.

Y el lector conocerá, también, que la relación entre ambos espacios es "holística", es decir, que el valor de dicha función en cada punto de la celdilla, de coordenadas (xyz) , es el resultado de "sumar" la contribución de **todos** los factores de estructura (haces de difracción) que muestra el espectro de difracción, que son muy numerosos (varios miles para una estructura sencilla, y cientos de miles para una estructura de una proteína).

El "salto" entre espacios directo y recíproco, mediado por la transformada de Fourier que representa la función de densidad electrónica

Además, el número de puntos en la celdilla en donde calcular la función ρ es muy elevado. Basta pensar que en una celdilla de unos $100 \times 100 \times 100$ Angstrom³ sería necesario calcular, como mínimo, 1000 puntos en cada dirección de la celdilla, para obtener una resolución de $100/1000=0.1$ Angstrom en cada dirección. Ello supone calcular dicha función, como mínimo, en $1000 \times 1000 \times 1000$ puntos = 1.000.000.000 puntos (mil millones de puntos) y en cada punto utilizar los varios cientos de miles de factores de estructura $F(hkl)$ del espectro.

Resulta, pues, evidente que al margen de las dificultades que encierra el **problema de la fase**, resolver una estructura cristalina implica la necesidad de medios de cálculo potentes.

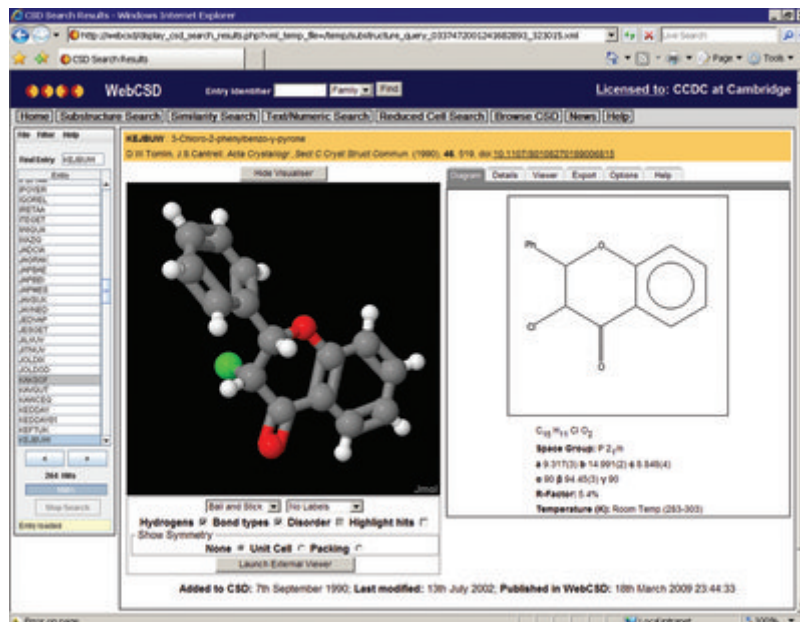
Finalmente, el análisis de una estructura implica, además, la necesidad de calcular toda una serie de parámetros geométricos que la definen, distancias interatómicas, ángulos de enlace, ángulos de torsión en los enlaces, superficies moleculares, etc., y para los que es necesario utilizar las coordenadas (xyz) de cada átomo en la estructura.

This new webpage has been designed to attract beginners to the fascinating world of Crystallography. Different chapters present fundamental concepts illustrated with many figures and animations. Topics include structure of crystals, X-rays, symmetry and lattices, scattering and diffraction (comparing old and recent experimental developments), structural resolution, the meaning of the structural model, computing, etc., without forgetting its historical context. Moreover, these web pages are offered in both English and Spanish.

NOTICE

WebCSD: Fast web-based access to the latest crystal structures

www.ccdc.cam.ac.uk/products/csd_system/webcsd



Search result showing 3-chloro-2-phenylbenzo[d][1,3]dioxole (CSD refcode KEJBUW); the 3D structure can be manipulated within the embedded visualiser (Jmol).

The CCDC is pleased to announce that internet access to the Cambridge Structural Database (CSD) will soon be available.

WebCSD has been developed using CCDC's C++ toolkit and enhances the search, analysis, exploration and validation tools already provided with the CSD System. The software searches on a relational SQL version of the CSD and affords convenient and rapid access to this unique database that is approaching one-half million crystal structures.

Convenient and rapid access: WebCSD does not require you to install and register software locally; institutions with a site-wide CSD licence need only to provide their IP range(s) and the CSD can immediately be searched or browsed from any computer across their entire site. Automatic software and database updates: Database updates will be made regularly providing you with access to the very latest structures. In addition, new features can be made available as soon as they are developed.

Searching and browsing results: WebCSD has been designed with speed, simplicity and convenience of use in mind. In addition to offering a full range of text, numeric and bibliographic search options, WebCSD provides reduced cell, 2D substructure, and similarity search options. Search results are displayed in your browser. This convenient new display offers a choice of embedded 3D visualiser: Jmol or AstexViewer. All crystallographic information for a hit structure is presented in a single tabbed pane, including a 2D chemical diagram. Furthermore, selected text fields are hyperlinked allowing immediate retrieval of all other CSD entries containing a particular keyword e.g. *plate*, *cyclopentadienyl*, *Allen*.

Use in teaching: With WebCSD teachers obtain a tool that will have great value in the classroom. A range of illustrative teaching exercises that utilise WebCSD are available on the CCDC website: http://www.ccdc.cam.ac.uk/free_services/teaching/. WebCSD used in conjunction with these teaching materials will help make crystallographic data accessible to the non-specialist. This provides opportunity to

showcase the power of crystallography as a technique to a broad audience, and to demonstrate the utility of crystallographic information across the whole of the chemistry curriculum.

Gary Battle