

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



William L. Duax

The guiding principles of the IUCr include advancement of structural science, bringing structural science to emerging nations, and training young crystallographers for the future. The African Initiative of the European Crystallographic Assn (ECA), a Regional Affiliate of the IUCr, has been a model application of these principals. Thanks to the leadership of Jan Boeyens, Henk Schenk, and Claude Lecomte, Algeria, Morocco, Cameroon, Kenya, and Tunisia are, or soon will be, members of the ECA and may soon join Egypt and South Africa as full members of the IUCr.

Andre Roodt, Demi Levendis, and the Crystallographic Assn of South Africa took a giant step in drawing international attention to the high caliber of crystallographic research on the African continent by inviting the ECA to hold its 21st annual meeting in Durban in 2003. It is a tribute to the ECA that they took the risk of holding their meeting so far from the center of their member population. I was pleased to be able to participate in this meeting, the first to be held on the African Continent.

The American Crystallographic Assn (ACA) has followed the example of the ECA in developing a Latin American Initiative, working together with leading laboratories in Brazil, Venezuela, Argentina, Mexico, and other Latin American countries to strengthen the crystallographic infrastructure there.

Before going to Africa, I attended the meeting of the Asian Crystallographic Assn (AsCA) in Broome, Australia. The meeting, held jointly with the meeting of the Crystallographic Assn of Australia and New Zealand (SCANZ), attracted 350 crystallographers from throughout the Asian region and covered all areas of crystallography.

The Executive Committee of the IUCr has often convened one of their business meetings concurrent with an ECA meeting and occasionally with an ACA meeting. This year for the first time, the Executive Committee held its annual business meeting at the site of an AsCA meeting in Broome, Australia. The major actions taken by the Executive Committee at that meeting include the following:

- The Program Committee for the Florence 2005 Congress was approved. After much careful consideration, Carlo Mealli, the Program Chair, proposed a 21-member committee with representation from all the IUCr Commissions. The members of the committee are listed on Page 23. Suggestions for microsymposia topics, plenary lecture topics and speakers, and session chairs are invited from individuals as well as all national committees.
- The Ewald Committee has been selected. Michiyoshi Tanaka of Japan, a former member of the Executive Committee has agreed to chair the committee. The other 6 members of the committee will be announced in the *IUCr Newsletter* once they have accepted the invitation. Rules concerning nomination for the Ewald Prize will also appear in the *IUCr Newsletter* and on the IUCr website. The membership of the Florence Program Committee and the Ewald Committee reflect a wide range of crystallographic expertise, as well as geographical and gender balance.
- A plan for the development of a 2nd electronic journal, *Acta Cryst F*, a macromolecular analogue of *Acta E*, was approved. *Acta F* will cover crystal growth and protein genomics.
- Hartmut Fuess of Germany was appointed as the new Chairman of the Commission on International Tables, an appointment critically important to the development of new Tables tailored to the needs of our rapidly growing, and highly diversified community.

- The financial health of the Union is good and the budget allocation for the calendar committee was increased to allow expanded support for student participation in the meetings of regional affiliates, their satellites and intercongress meetings. Countries that have never applied for support should plan to do so. Instructions are on the website.
- The Committee reviewed a proposal for expansion of the composition of the Executive Committee and the procedures for elections proposed by the Past President of the British Crystallographic Assn. The proposal will appear in a future issue of the IUCr Newsletter and may be a topic for discussion and action at the Congress in Florence.
- This issue of the *IUCr Newsletter* includes a comprehensive review of crystallography in Latin America prepared by Executive Committee member Iris Torriani. Similar reviews concerning crystallography in Italy by Davide Viterbo, in Germany by Gernot Heger, in Russia by Leonid Aslanov, in Japan by Yuji Ohashi, and in China by Ze Zhang will appear in future issues. The Newsletter Editor welcomes articles about crystallography in other countries in the Union or its Regional Affiliates.

The Executive Committee voted to inaugurate a new series of IUCr awards to be presented at meetings of the regional affiliates and national crystallographic associations. The prizes include on-line subscriptions to Acta journals, copies of *Crystallography Across the Disciplines* and other IUCr publications. The Executive Committee advocates the awarding of these prizes to undergraduate or graduate students or crystallographers beginning a teaching career, but the final decision will be up to the meeting organizers. The first of these prizes were awarded at the AsCA meeting in Broome, the ECM meeting in Durban, South Africa, and the satellite, INDABA IV.

It is my opinion that the greatest strength of the IUCr in the next 50 years will come from emerging nations in South America, Africa, and Asia – countries rich in natural resources, new ideas, and bright young people. International communication and cooperation fostered by organizations such as the IUCr are the best tools with which to combat terrorism, ignorance and intolerance. Only education will empower people of all nations, making it possible for them to use their natural resources to improve their lives and promote peaceful coexistence and cultural and religious tolerance among all nations.

I ask all of you to assist me and the members of the Executive Committee of the IUCr and the Commissions of the Union to work to achieve the goals of our union. Please feel free to speak to or write to me or other members of the Executive Committee about your concerns and how the Union can better serve you. Most of all, help us to extend the benefits of the Union to nations not currently members.

LETTER TO THE EDITOR

In response to the President's letter (Vol. 11. No. 2, 2003)



Members of the IUCr Executive Committee met in Broome, Australia. Bottom row (left to right): Xe Zhang, Sine Larsen, Iris Torriani, Bill Duax, back row: Leonid Aslanov, Gernot Heger, Yuji Ohashi, and Davide Viterbo.

Dear Bill,

Complaints from under-represented countries are nearly as old as the IUCr itself. I met them several times when I served as General Secretary-Treasurer from 1972-1981. Colleagues with long-term involvement in Union affairs told me that complaints of under-representation went a long way back both of membership of Commissions and of the Executive Committee. It appears that some Delegates to the General Assembly associated membership of Executive Committee and Commissions with national prestige.

I believe that it cannot be emphasised strongly enough that Officers of the Union and Commission Members are elected by the General Assembly and therefore represent **all** crystallographers and not any specific country. They are elected to serve their fellow crystallographers with their particular skills. Not to enhance the prestige of a country. I have received criticism from Delegates because their countries were not being represented on any Commission in spite of the fact that they had not nominated any person for membership.

Ideally, crystallographers from all member countries should participate in Union affairs to make it a truly International Union but it is up to the National Committees to bring names of talented and willing crystallographers to the Executive Committee and Commission Chairpersons.

There is another kind of under-representation that I would like to bring to attention. In 1972 the General Assembly elected its first and so far only female President : Dorothy Hodgkin. But, at the same occasion very few women were elected members of Commissions and several had no female members at all, in spite of the fact that crystallography has almost always recruited a higher percentage of women than most other physical sciences. Fortunately, the number of women on Commissions has since increased and the Union has a highly competent and respected female General Secretary-Treasurer.

But why is a Nobel Prize apparently a prerequisite for a woman to be elected President but not for a man? (J. Karle was elected President before he got the Nobel Prize).

Please do not get me wrong. I consider all elected Presidents of the Union fully worthy of their office, but as there are many highly estimated female crystallographers in our science, I hope that we shall see another female President in a not too distant future.

Svend Erik Rasmussen, U. of Aarhus, Denmark

Dear Svend,

Thank you very much for your letter. It is important to be reminded that the elected members of the Executive Committee and Commissions represent all crystallographers. Nevertheless, I too think that 'Ideally, crystallographers from all member countries should participate in Union affairs...'

My concern that representation on commissions have a wide geographic range is not motivated by a desire to lend prestige to any country, but a desire to enhance meaningful involvement by all countries. We are an International Union and our union will be stronger if all nations participate fully at all levels.

I have been gathering information on the structure, composition and policies of the National Committees. In some cases National Committees have had no change in membership for six years or more, cannot remember when they last met, and are uncertain of their responsibilities. The newsletter provides a way of sharing information and raising issues, with thousands of crystallographers around the world that may help to revitalize the Union.

As to the question of a woman president, I could not agree with you more. I am very pleased that there are three women on the Executive Committee at the present time. When I chaired the Program Committee for the Seattle Meeting, I included many women on the committee. (At that time I was told by some members of the Executive Committee that it was not necessary to have women on the committee because the composition of the Program Committee should be based on scientific merit only and not gender.)

It is also encouraging that the current president of ASCA and the president elect of the ACA are both women. (The ACA has had six women presidents in the past 16 years.)

Bill Duax

EDITORIAL

Guest editorial - Carlo Mealli



This is my 35th year in the world of crystallography and structural chemistry. When I started, the discipline was just beginning to flourish. The first computers and diffractometers, together with new methods of crystal structure determination, were giving a tremendous boost to the development of modern chemistry (organic, inorganic, organometallics, solid state, biological, etc.). Indeed, during my working years, the Cambridge Structural Database has grown from a few thousand to about 300,000 entries. It is therefore no exaggeration to say that crystallography has provided the underpinning for much of structural chemistry. My personal scientific journey has also brought me into the realm of computational and theoretical chemistry. These tools are very important for the interpretation of molecular structure and chemical bonding. In this area, I had the unique and invaluable good fortune to collaborate with Roald Hoffmann, Nobel laureate in chemistry in 1981. From him, I learned how powerful the analysis of a phenomenon is by seeking its relationships with other phenomena of equal complexity. Such a '*horizontal*' approach provides a counterpoint to the reductionist mode of understanding that makes a '*vertical*' excursion through the hierarchy of the sciences (literature and social sciences would be explained by biological functions, biological ones by chemical ones, chemistry by physical laws and the latter by mathematics). Structural chemistry is perfectly suited to the horizontal way of thinking as the most subtle geometrical diversity can explain different chemical properties and behaviors (R. Hoffmann, *The Same and not the Same* Columbia University Press, 1995).

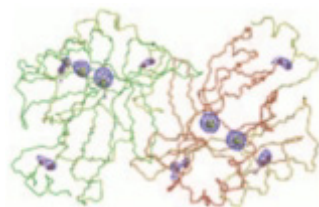
For a long time I have enjoyed discussions at crystallographic meetings with colleagues who use their insight to infer chemical properties from the 3D arrangement of molecules. Today, molecular structure is still the basis for any serious chemical study (consider, in this respect, the constantly increasing number of diffractometers sold world-wide). On the other hand, one may have the impression that the molecular crystallographer, once a main actor, is now a species doomed to extinction, rarely encountered at crystallographic conferences. Conversely, it is true that crystallographers, including those who provide structural results as a service and the chemists who solve their own structures, are the source of a tremendous amount of precious data that may be correlated. This is also the reason why I was one of the proponents of the Special Interest Group on 'Molecular Structure and Chemical Properties' within the European Crystallographic Assn.

When I accepted the honour and responsibility of organizing, the XXth IUCr congress together with other Florentine colleagues, not only did I want to demonstrate my still intact love for the discipline, but I also made a special promise. In addition to assembling a high level scientific program on all the multidisciplinary aspects of crystallography, I would like to revitalize the participation of the wider community of chemical crystallographers and structural chemists. In particular, I expect that Florence, the historical city of the Renaissance, will stimulate again discussions on structural problems in the most appropriate framework of the world congress. Finally, I want to reassure all crystallographers that even now, two years before the congress, the Florentine community is already deeply involved in the organizational details. Our primary goal is to provide a successful and unforgettable Congress.

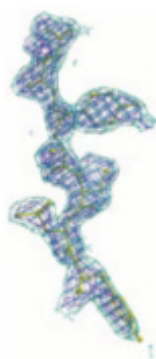
IUCR JOURNALS NEWS

S-SWAT (softer single-wavelength anomalous technique): potential in high-throughput protein crystallography

***Acta Cryst.* (2003). A59, 327-334**



Overview of apocrustacyanin A1 dimer and anomalous difference Fourier electron density map. Xe atoms are coloured in yellow; disulfide bridge sulfurs are in orange.



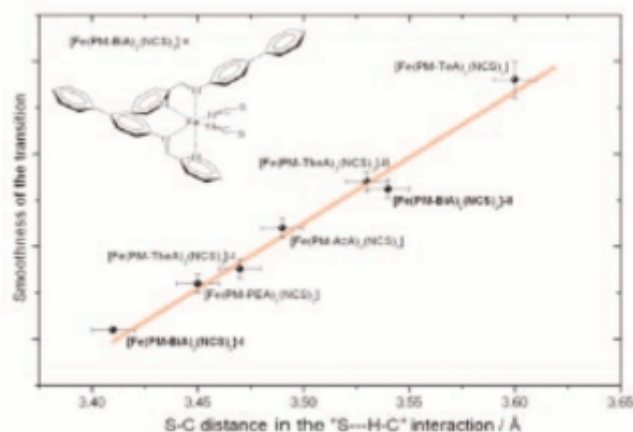
An example of the quality of the electron-density portions (phases from *MLPHARE/DM*, $2F_o - F_c$, 2 r.m.s.) overlaid on a fragment of the main chain of apocrustacyanin A1.

The drive for higher output of protein crystal structures sustains an interest in streamlining protocols. Synchrotron radiation beamlines offer automated data collection with faster and larger detectors, choice of wavelength(s), intense beams and fine collimation. Presented here is a single-wavelength approach 'Softer-SWAT' exploiting the large optimized f' signal of the Xe *L*1 absorption edge, and producing *de novo* phases. A high-quality electron-density map was obtained when phase improvement methods were used. This approach may also harness the iodine optimized f' and enhanced sulfur f' signals. This case study contributed to the design of the new Daresbury SRS Multipole Wiggler Beamline 10. It also led to the development of a new formula to evaluate the anomalous signal of multiple anomalous scatterers in protein crystals.

A. Olczak, M. Cianci, Q. Hao, P. J. Rizkallah, J. Raftery and J. R. Helliwell

Towards direct correlations between spin-crossover and structural features in iron(II) complexes

Acta Cryst. (2003). B59, 479–486



Smoothness of the spin transition extracted from the magnetic curve versus the S–C distance of the S···H(C) intermolecular hydrogen interaction from the crystal structure.

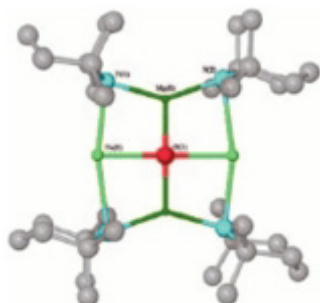
The spin crossover $[\text{Fe}(\text{PM-BiA})_2(\text{NCS})_2]$ complex, where PM is *N*-(2-pyridylmethylene) and BiA 4-aminobiphenyl, can crystallize in two polymorphs. The orthorhombic phase undergoes a very abrupt spin transition at $T_{1/2} = 167$ K while the monoclinic phase undergoes a gradual spin transition at $T_{1/2} = 205$ K. The polymorphism of this compound has been used to underline the structural properties responsible for such a difference in the magnetic behavior. New structural parameters are defined, and directly linked to the magnetic properties, in particular the cooperativity of the spin transition. The results are extended to all the complexes belonging to the same family of general formula $[\text{Fe}(\text{PML})_2(\text{NCS})_2]$. In this family, the spin-transition features are driven by weak intermolecular interactions such as S···H(C) hydrogen-like contacts.

M. Marchivie, P. Guionneau, J.-F. Létard and D. Chasseau

IUCR JOURNALS NEWS

A 'missing' member of the inverse crown ether family

***Acta Cryst.* (2003). C59, m302-m303**

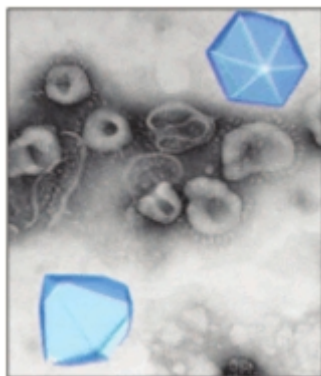


Inverse crown ethers are so called as they reverse the normal roles found in crown ethers, with a positively charged s-block metal based ring capturing O, C or H based anions at its core. These materials are of great interest to synthetic chemists as they selectively (and often multiply) deprotonate a range of organic substrates including the aromatic rings of metallocenes and arenes. In the absence of appropriate substrates, inverse crown ethers act as efficient oxygen scavengers. In this paper it is shown that a previously unknown Na/Mg example with an oxide core can be synthesized by blocking the alternative aromatic metallation route *via* the use of sterically hindered 1,3,5-mesitylene as solvent.

Alan R. Kennedy, Jonathan G. MacLellan and Robert E. Mulvey

Structural genomics of the SARS coronavirus: preliminary crystallographic study of the Nsp9 protein

***Acta Cryst.* (2003). D59, 1628-1631**



Optimized crystals of the SARS-CoV Nsp9 protein. An electron microscopy view of a coronavirus is displayed in the background (courtesy of Prof. McNulty, Queen's U., Belfast, UK)

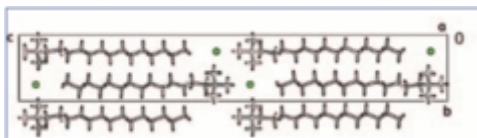
The recent epidemics of Severe Acute Respiratory Syndrome (SARS) represent a real paradigm for emerging viral pathogens. The etiologic agent of SARS (SARS-CoV), a positive-stranded RNA virus within the Coronaviridae family, is mainly transmitted by the respiratory route. In the absence of any efficient treatment, a wide effort is being made to design drugs against this agent. In this context, we have developed a SARS-CoV whole genome approach aimed at determining the crystal structure of all the 28 SARS-CoV proteins. We anticipate that this will greatly facilitate drug design and contribute to fundamental knowledge. The SARS-CoV genome encodes two large replicase polyproteins, which are processed into a set of mature non-structural proteins by internal viral proteases [E. J. Snijder, P. J. Bredenbeek, J. C. Dobbe, V. Thiel, J. Ziebuhr, L. L. M. Poon, Y. Guan, M. Rozanov, W. J. M. Spaan and A. E. Gorbalenya (2003). *J. Mol. Biol.* **331**: 991-1004]. We have crystallized one of the replicase proteins (Nsp9, 113 residues), which diffracts to 2.8 Å resolution.

Valérie Campanacci, Marie-Pierre Egloff, Sonia Longhi, François Ferron, Corinne Rancurel, Aurelia Salomoni, Cécile Duroseau, Fabienne Tocque, Nicolas Brémond, Jessika C. Dobbe, Eric J. Snijder, Bruno Canard and Christian Cambillau

IUCR JOURNALS NEWS

Pseudosymmetry in tetradecyltrimethylammonium bromide

Acta Cryst. (2003). E59, o1151-o1152



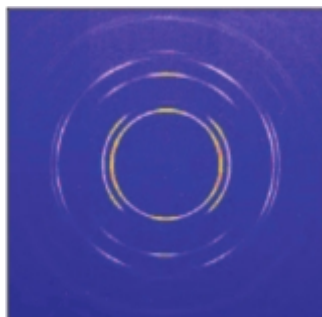
Tetradecyltrimethylammonium bromide is commonly used as a surfactant and germicide. A single crystal grown serendipitously from the residual detergent used to wash laboratory glassware was analyzed showing that the long organic molecules are packed in layers with the tetradecyl chains adopting an extended zigzag form. These long chains are parallel within a layer and antiparallel in alternate layers. This packing emulates a c -halved unit cell in space group $P2_1/m$, but it is not supported by the diffraction data, as many reflections with $l = 2n + 1$ showed weak, but significant, intensity. Refinement in the half cell in $P2_1$ or $P2_1/m$ resulted in unrealistic bond lengths and displacement parameters. Including all the data and refining in space group $P2_1/c$ revealed the true structure.

M. Ramos Silva, A. Matos Beja and J. A. Paixão

IUCR JOURNALS NEWS

Synchrotron texture analysis with area detectors

***J. Appl. Cryst.* (2003). 36, 1040-1049**

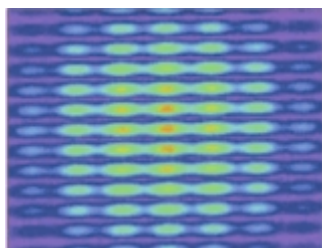


Intensity variations along Debye rings on synchrotron diffraction images, as that of rolled copper measured during recrystallization at ESRF, immediately reveal crystallite preferred orientation. This is problematical to structural crystallographers who need true diffraction intensities, but of great interest to those concerned with anisotropic material properties. The article addresses both issues by demonstrating a method to determine the quantitative orientation distribution from single images, with algorithms from tomography. The orientation distribution can then be used to normalize intensities and to calculate textural characteristics. This method is being refined to process images directly with the Rietveld approach, allowing simultaneous retrieval of structural, textural and microstructural parameters.

H.-R. Wenk and S. Grigull

Two-dimensional visible synchrotron light interferometry for transverse beam-profile measurement at the SPring-8 storage ring

J. Synchrotron Rad. (2003). **10**, 295–302



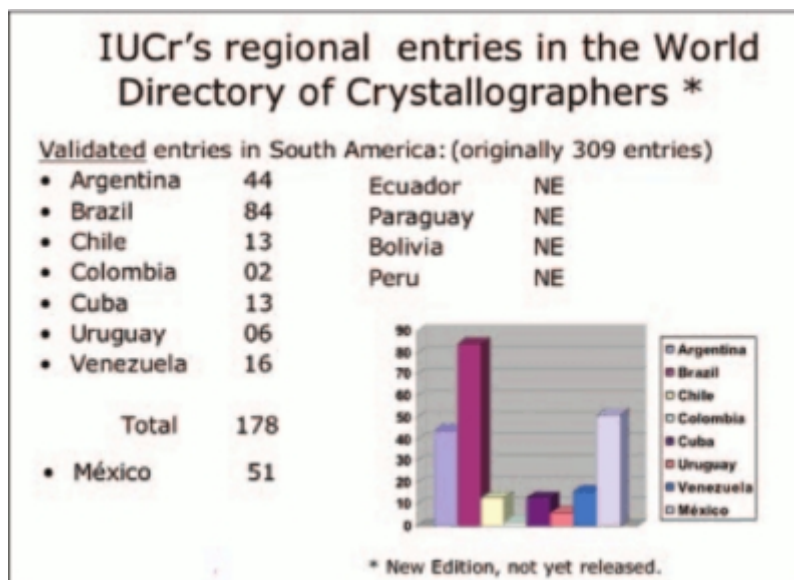
Observed two-dimensional interference pattern at the working point (ν_x, ν_y) = (40.15, 18.35) close to the condition for users' time operation.

Emittance of an electron beam, which is inversely proportional to the brilliance of the synchrotron radiation, is one of the most important characteristics of a storage ring operated as a synchrotron light source. We have recently developed a two-dimensional visible synchrotron light interferometer for nondestructive measurement of the transverse beam profile giving us information about the emittance. The interferometer has two times better resolution than the conventional beam-imaging monitor. The point-spread function of the interferometer can be calibrated experimentally. The two-dimensional profiling capabilities were verified by observing an electron beam stored in the SPring-8 storage ring operated at various working points. Beam-size broadening and beam tilting were clearly observed near the differential and sum resonance conditions.

M. Masaki and S. Takano

SPECIAL REPORT

Crystallography in Latin America



Several countries have been very active in the development of crystallography in South America since as early as the 1940s. Ernesto Galloni, who can be considered one of the pioneers of crystallography in Argentina, and in Latin America, used to describe his first attempts at performing X-ray experiments at the Cancer Inst. in Buenos Aires using completely inadequate X-ray generators.

In 1959 UNESCO financed a Latin American course on Pure and Applied Crystallography in Santiago, Chile, chaired by the Spanish crystallographer Julio Garrido. On this occasion, the idea of forming a group that would unite all the crystallographers of Ibero American origin was conceived.

The first meeting of the Grupo Iberoamericano de Cristalografía took place in 1960 in the city of Córdoba, Argentina. Their charter was signed by crystallographers from Argentina, Chile and Spain (M. Abeledo, M.R. Benyacar, S. Caticha Ellis, E. Galloni, D. Garaycochea, A. Joel and O. Wittke).

The second meeting of the Grupo Iberoamericano de Cristalografía took place ten years later in Buenos Aires, July 8-16, 1970. It was organized by J. Garrido, L. Brú, M. Font Altaba, J.R. Martínez, all from Spain, and E. Galloni, M. Abeledo, A. Bonfiglioli, C.R. Cortelezzi and M. Iñiguez from Argentina. At this meeting, there were contributions from Argentina, Brazil, Chile, Uruguay, Venezuela and Spain.



In 1975 a meeting of the Ibero-American Group in Campinas, São Paulo, Brazil attracted more than 200 participants from most of the South American countries, Spain and Portugal. Successive meetings were organized in Buenos Aires, Chile, Portugal and Mexico. In 1990 the Ibero-American Group met in Mérida, Venezuela. At this meeting and at subsequent meetings in Madrid, Spain (1992) and Montevideo, Uruguay (1994) a satellite school on crystallography was organized, sponsored by the IUCr. Unfortunately, the hardships of modern economies in the countries involved presented great difficulties to the organizers of these meetings, and the contacts and links that sustained the organization were broken.

A survey based on the present information available from the groups in South America shows that crystallography is still an important part of scientific research in several countries. We note that several countries are not represented in the World Directory of Crystallography, including Ecuador, Peru, Bolivia and Paraguay. However, there are some university X-ray diffraction labs in those countries, mainly dedicated to materials science research using crystallographic methods.

Over the years, the World Directory of Crystallographers has become a very important tool for identifying researchers involved in all areas of crystallography in all countries. At present, its electronic format makes registration quite easy. But when we look at the list, we are somewhat disappointed. The number of Latin American crystallographers registered is smaller than expected (309 entries). Reasons for this are probably the lack of adequate internet facilities in the Latin American countries and reluctance of people to identify themselves as crystallographers!



This is not a complete listing of the groups in each country, since information keeps coming, and it will take time to identify all existing groups. From the Central American countries we would like to mention Cuba, whose crystallographers have been registered in the WDC and have participated in the IUCr congresses for more than twenty years. At the moment they are a small group, but still interact significantly with México, Brazil, Colombia and Venezuela. Other Central American countries, such as Puerto Rico, Costa Rica and Panamá, although active in research, have not interacted with other Latin American crystallographers to the best of our knowledge.

For Crystallography in Brazil, a very important landmark was a School on Direct Methods organized by Y. Mascarenhas in São Carlos in 1974. The presence of several distinguished crystallographers, P.P. Ewald, J. Karle, H. Hauptman and M. Woolfson, attracted a number of participants from other Latin American countries. The school was the starting point for the formation of the Brazilian Crystallographic Assn (SBCr), affiliation to the IUCr, and nomination of a National Committee. X-ray diffraction as a tool for structural research had already been started in several institutions, but the creation of the Crystallographic Society was instrumental in organizing meetings and establishing connections among the different groups in the country.

Nowadays, there are approximately 12 well established groups in Brazil, working in different areas of crystallography, in universities and research institutions. The labs are described in the accompanying article.

The Nat'l Synchrotron Light Lab in Campinas, Brazil, since its inauguration in 1997, has been making great efforts to make its facilities available to Latin American researchers. A summer school program was created several years ago and has been very successful, attracting undergraduate students from Central and South America. The scholarships offered cover all expenses for two months. Latin American conferences are organized quite frequently, covering the most recent and important scientific subjects. The Nat'l Synchrotron Light Lab also organizes a users meetings every year, and this event is frequently a good occasion to bring together researchers from several Latin American countries.

In other countries, like Venezuela and Colombia, several crystallography groups were formed at approximately the same time in the 1980s. In Venezuela, a crystallographic society was formally registered in 1992, but it is not currently active. There is an effort going on to revitalize the Society. Some researchers take advantage of the Nat'l Conventions of the Venezuelan Assn for the Advancement of Science (ASOVAC) to gather for discussions. The labs or groups working in crystallography and X-ray diffraction are the following: three main satellites of the Lab Nacional de Difracción de Rayos X (LNDR-X) are located at the Universidad de los Andes, Mérida, the Inst. Venezolano de Investigaciones Científicas (IVIC), Caracas and UNEXPO, Puerto Ordaz. In addition, other groups have been active for many years at the Universidad Central de Venezuela, the Universidad Simón Bolívar, the Centro de Biofísica y Bioquímica (IVIC) and the Inst. de Tecnología (IUT) in Caracas. There is another group at the Universidad de Oriente, Cumaná. In all, a total of nine main groups and 10 associated groups (using the instrumentation in the main labs) were reported in Venezuela.

Throughout the 90s, several schools and meetings were organized in Venezuela, covering several aspects of crystallography. Some of them had the sponsorship of the IUCr and the ACA. Very dynamic and motivated, the groups mentioned above are the main representation of Venezuelan crystallography. They have no National Committee and affiliation to the IUCr is maintained thanks to the efforts of several groups.

From Oscar Wittke, Santiago de Chile, we learn that crystallography was started in Chile in 1952, when the Crystallography Lab of the Facultad de Ciencias Físicas y Matemáticas of the University of Chile was installed, and it has been functioning for over 50 years. Today, Chile maintains its affiliation to the IUCr, started in 1954. There is a National Committee of Crystallography, but a Crystallographic Society has never has been established. The groups that are more active at the present time are located in three Universities in Santiago, Antofagasta and Concepción. This last group is involved in biophysical applications, and small angle diffraction. One of the labs in Santiago and one in Antofagasta are more dedicated to materials science and engineering.

Uruguayan scientists dedicated to crystallography have participated in the activities of neighboring countries since the early 70s, as part of the Ibero American group. There is no record of their affiliation to the IUCr or of the existence of a crystallographic society. Within this small country they have created several groups related to the only public university in Uruguay (Universidad de la República), in the Schools of Chemistry, Engineering and Science. According to recent reports, current crystallographic interests are crystal growth, applications in solid state physics and structural chemistry using single crystal instrumentation, a powder diffractometer, and a crystal growth lab.

In Argentina, the crystallographers that organized the meetings with the Ibero-American Group in the 1960s and 1970s, belonged to the University of Buenos Aires, the Atomic Energy Commission (CNEA), in Buenos Aires, and the University of Cordoba. New centers were later developed at the Atomic Center in Bariloche, Universidad de La Plata, Universidad del Litoral and Universidad del Sur. Labs for the characterization of materials and solid state applications are notably those of Cordoba (Ceprocór), Universidad Nacional del Sur-Santa Fé, CNEA-Buenos Aires, Centro de Investigaciones en Sólidos

(CITEFA)-Buenos Aires, LANADI-La Plata and CNEA-Bariloche. In La Plata, there is infrastructure for the study of small molecules. At CNEA-Buenos Aires, there is also a diffractometer (a donation from the UK) used for this purpose. A group of young researchers have recently installed a laboratory at the Leloir Institute in Buenos Aires that will be dedicated to protein crystallography. Other groups at the Universidad Nacional de San Luis, Universidad Nacional de Misiones and Universidad Nacional de la Patagonia are also part of the Argentinian community. A detailed list includes 19 groups, not all of them having complete infrastructure for their research.

Although Argentina produced many competent crystallographers, they too often left the country and never found favorable conditions to return. The groups existing today struggle to work in difficult conditions. Since the time of its affiliation to the IUCr, there has been a National Committee for Crystallography in Argentina as well as an Argentinian Crystallographic Assn. Nowadays, some young crystallographers are trying to revitalize the Crystallographic Society, and have already nominated a National Committee. There are good prospects for the rejuvenation of the enthusiasm of the past in Argentina.

According to the Secretary of Relations of the Mexican Society of Crystallography (SMCr), A.R. Arellano. The SMCr was founded in 1995 and a Nat'l Committee has been appointed. The SMCr has more than 500 members involved in crystallographic research in several areas, most of them from chemistry and physics, but geology and biology are also represented. Society meetings take place every three years, and schools and courses are organized in different cities every year. These events, designated as 'Crystallography Week' are intended to promote the nationwide teaching of Crystallography. Mexico is affiliated to the IUCr. Several mexican groups have visited Brazil during the past three years, with the purpose of performing experiments at the Brazilian Synchrotron Light Source and also participating of Inter-American events. This very desirable interaction is much needed, a fact well understood by the several institutions that have established exchange programs, like the Centro Latino Americano de Física (CLAF), Nat'l Science Foundation (NSFIGERT) and the American Physical Soc. (APS).

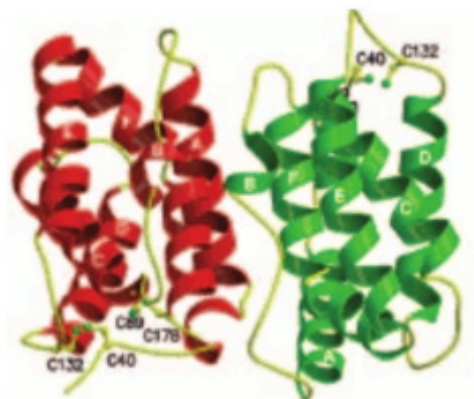
As stated before, many details may have been overlooked in this report. It should be considered the first installment of a future review, which will be written when more information reaches us to complete the picture of the crystallographic community in Latin America.

Iris L. Torriani

Thanks are due to the following Latin American crystallographers for some of the information contained in this report: Daniel Vega and Graciela Punte (Argentina), Yvonne Mascarenhas (Brazil), Oscar Wittke (Chile), Graciela Delgado (Venezuela), Laura Fornaro (Uruguay), Alicia R. Arellano (México). Comments and new information on the subject can be sent to torriani@ifi.unicamp.br and will be greatly appreciated.

SPECIAL REPORT

Crystallography in Brazil



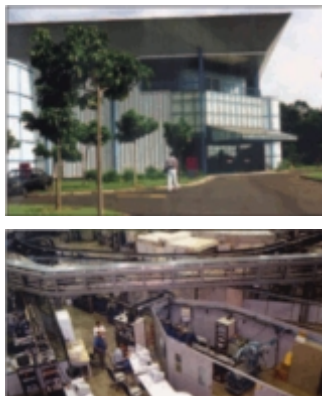
Crystal structure of Recombinant Human Interleukin-22. R.A.P. Nagem *et al.*, *Structure*, Vol **10**, 1051-1062, August 2002.

A survey of the Brazilian groups dedicated to crystallography showed a variety of interests, dealing with material science and biological research. X-ray diffraction is the main experimental tool and consequently X-ray laboratories are equipped with conventional sources and the instrumentation necessary for the different techniques and applications. These groups, are mainly associated with universities and research institutes. Brazil also has a synchrotron light source at the Nat'l Synchrotron Light Source (LNLS), the only such facility below the equator, and a neutron reactor at the Nat'l Inst. for Nuclear Research (IPEN). A brief description of the main crystallography groups in the country is given below.

National Synchrotron Light Laboratory / Laboratório Nacional de Luz Síncrotron (LNLS), Campinas, São Paulo, Brazil



This is the largest experimental facility for the use and development of X-ray techniques not only in Brazil but in all of Latin America. It provides access to researchers from any country, and especially from all of South America. Several beamlines operate in the soft and hard X-ray wavelength region, and beamtime is allocated by peer review of projects submitted by the users.



The 1.37 GeV electron ring of the LNLS has been in operations since July 1, 1996.

Experimental stations used in crystallographic research presently in operation are: Protein Crystallography (PCr), X-ray absorption (EXAFS, DXAFS), Soft X-rays (SXS), small angle scattering (SAXS),

powder diffraction (XRD), multiple axis single crystal X-ray diffraction (XRD1), and 6-axis single crystal X-ray diffraction (XRD2).

A new protein crystallography beamline will be installed shortly. This will be a wiggler beamline for MAD experiments. A second small angle scattering beamline SAXS2 and a new EXAFS beamline are under construction.

At present the LNLS staff is formed by a group of approximately 20 researchers in different areas, which include, apart from the SR facilities, a high resolution NMR Lab and the Structural Molecular Biology Lab, which are also national facilities associated to the LNLS, installed in the same campus, offering infrastructure to external users.

University of Campinas (Unicamp) / Applied X-ray Crystallography Laboratory - Physics Institute, Cambinas, São Paulo, Brazil



The Applied X-ray Crystallography Lab of the Physics Inst., Unicamp started its activities in 1974. It is equipped with several conventional X-ray sources, and the main research interests are:

- Small Angle X-ray Scattering of macromolecules;
- High resolution single crystal diffraction;
- Thin films and multilayers and heterostructures;
- Powder diffraction (high and low temperature studies, Rietveld refinement);
- Diffraction from magnetic materials.



The group has three researchers and four PhD students and maintains a close interaction with the Synchrotron Lab.

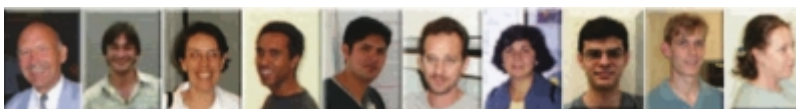
Contact: torriani@ifi.unicamp.br.

University of São Paulo (USP), Physics Institute, São Paulo / Universidade de São Paulo , Departamento de Física Aplicada - Instituto de Física, Grupo de Cristalografia



The USP-São Paulo Crystallography group was established in the early 70s. At present it is involved in the following lines of research: materials science and interdisciplinary topics especially related to structural problems, like the study of semiconductor crystals, films and surfaces, epitaxial growth, liquid crystals, gels and complex fluids. The main techniques used are single crystal diffraction, powder diffraction and

small angle scattering. Special attention is given to research in materials used in opto-electronic devices and in complex systems with supramolecular order.



The group has 5 researchers and several graduate students.

Contact: mfantini@if.usp.br, cristalografia@pagina.de.

National Institute for Nuclear Research, São Paulo



The goal of the Institute is to develop scientific research and provide services using the Nuclear Reactor IEA-R1 as a source of neutrons and gamma radiation, generating scientific and technological knowledge, contributing to human resources development and to the improvement of the quality of life of the Brazilian population.

A major program to upgrade the diffractometer installed at the beam-hole N°6 of the reactor was undertaken from 1999-2000. The project, in collaboration with the Missouri university research reactor (MURR) includes 9 position sensitive detectors (PSD), a rotating-oscillating collimator and an elastically bent silicon single crystal monochromator. The PSD stack will allow simultaneous measurement of neutron intensity in an angular interval of 30° and the monochromator will permit the choice of three different neutron wavelengths. The combination of monochromator and PSD will lead to a considerable improvement in the spectral resolution and its data collection efficiency over the existing configuration.

University of São Paulo (USP), Physics Institute and Chemistry Institute, São Carlos, SP



Two Groups in the city of São Carlos are very active in several areas of Crystallography. They belong to the Physics Inst. and the Chemistry Institute of the São Carlos campus of the U. of São Paulo.



Main research areas are:

- Protein crystallography, for which the group has crystallization facilities. Main collaborations with other labs in São Paulo are: IBILCE/UNESP, São José do Rio Preto and LNLS, Campinas;
- Structure of small molecules;
- Powder diffraction of inorganic compounds, Rietveld refinement;
- Small angle scattering of organic and inorganic systems.

Six researchers are in charge of the different subjects, and a number of graduate students complete this important group.

Contact: oliva@ifsc.usp.br

University of São Paulo (USP), Geocigal Sciences Institute, São Paulo



The laboratories of the Geosciences Institute include X-ray fluorescence and diffraction routinely used for the characterization of rock minerals and soils. Powder diffraction techniques are used to investigate new structures.

Contact: igc@usp.br

Federal University of Goiás, Goiania, Go. - Physics Institute Laboratory of Crystallography and Materials



The main research activities of the Crystallography Lab of the Physics Inst. of the UFG were established a few years ago, and include: Physicochemical characterization of natural crystals, Crystal Growth (photo-refractive oxides and organic crystals with non-linear optical properties). Structure of organic and inorganic small molecules. The group consists of five researchers and several students.

Contact: lariucci@fis.ufg.br

University of Minas Gerais, Belo Horizonte, MG Physics Institute



The Crystallography group at the UFMG is involved in the following research activities:

- Study of incommensurate modulated structures;
- Intercalation compounds and metal complexes;
- Charge density studies of Hydrogen bonded compounds;
- Crystal structure, physical properties and cation distribution in minerals as spinels and perovskites.

Personnel: Two main researchers and graduate students.

Contacts: nspezial@fisica.ufmg.br, nelsongf@dedalus.lcc.ufmg.br

Universidade Federal De Brasilia, Instituto de Geociências



The U. of Brasilia is strategically located in the center of Brazil, in the country's capital. The Inst. of Geological Sciences was founded in 1965 with the aim of producing professional geologists so much needed in a country with enormous mineral resources. The Crystallography Lab in the IG has been active in the characterization of mineral samples using x-ray diffraction. The staff is composed of several researchers and graduate students.

Contacts: alva1@unb.br nilsonfb@unb.br

Federal University of Bahia UFba Physics Institute



For more than 20 years, the Crystallography Group of the UFba has been working in diffraction physics, study of the structure of epitaxial layers, and single crystals using self consistent theory and dynamical theory. Other subjects of interest are: multiple diffraction and X-ray topographic methods. Current projects are mainly theoretical.

Contact: dioni@ufba.br

Catholic University of Rio de Janeiro, RJ Materials Science and Metallurgy Department



The research group at the Materials Science and Metallurgy Dept of the PUC-Rio is engaged in the study of phase transitions in metallic alloys using temperature dependent XRD. The group is working in collaboration with researchers at Hasylab, Hamburg, and is involved in new imaging techniques in real time powder diffraction experiments.

Contact: rizzo@dfmm.puc-rio.br

Federal University of Paraná, Curitiba, Pr, Department of Physics, X-ray Optics Laboratory



This Lab has been of great importance in the development of instrumentation for the Brazilian Synchrotron Radiation Facility. Several researchers and graduate students are engaged in the following areas:

- High resolution diffractometry;
- Defects in single crystals;
- Grazing incidence technique;
- Thin films analyses;
- Diffraction at angles near $\pi/2$. X-ray topographic techniques;
- Development and construction of X-ray optical elements.

Contact: cusatis@fisica.ufpr.br



Other Labs in which X-ray diffraction facilities exist as research infrastructure of Applied Physics and Material Science Depts are located at the following institutions:

- Physics Institute, University of Santa Catarina (UFSC), Florianópolis, SC
- Physics Institute, University of Campinas, Campinas, SP
- Physics Institute, University of Rio Grande do Sul (UFRGS), Porto Alegre, RGS
- Centro Brasileiro de Pesquisas Físicas (CBPF), Rio de Janeiro, RJ



The participants of the last LNLS Annual Meeting

More information is being gathered to make this survey more comprehensive. Please send comments and additional information to torriani@ifi.unicamp.br.

Iris L. Torriani

SPECIAL REPORT

History of the Brazilian Crystallographic Association (SBCr)

History of the Brazilian Crystallographic Association (SBCr)



The SBCr was founded in 1971, during a School on Direct Methods in Crystallography at the San Carlos campus of the U. of São Paulo (USP). In those days, several researchers were making great efforts to establish experimental research labs in Brazil, and a group of them (12 geologists, 14 chemists, 21 physicists and 4 engineers) all working at several universities in the states of São Paulo and Rio de Janeiro, identified X-ray diffraction and structure analysis as their common field of research and founded the Sociedade Brasileira de Cristalografia (SBCr). The Society was established with a Provisional Council. The by-laws and goals were described in the charter of foundation, legally approved in 1976, when the first Administration Officers and Council were elected.



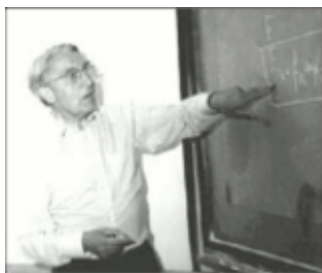
1974: Opening ceremony of a school on direct methods at the Physics Inst., USP-Sao Carlos, with the presence of a very prestigious group of lecturers: M.M. Woolfson, Jerome Karle, Isabella Karle, Edson Rodrigues, Sérgio and Yvonne Mascarenhas (organizers of the school), H. Hauptmann, P.P. Ewald, P. Main and L. Lessinger.

The eclectic origin of the founding members of the SBCr reflected the diversity of interests of the research groups in the early seventies, which is in essence the same that exists today in Brazil. The active crystallography groups in Brazil nowadays are devoted to very different areas of research, having in common the basic techniques of crystallography.



1985: Dorothy Hodgkin was in Campinas presiding at a Pugwash Conference. She found out there was a crystallography lab at the U. of Campinas, and she wanted to know us! Left to right: I. Torriani, C.F. Souza, M. Fantini, S. Caticha Ellis.

One of the main activities of our crystallographic society is the organization of bi-annual meetings, which attract researchers from several areas. In general, the number of participants is much larger than the number of active members, since new crystallographic methods and techniques are considered of direct application in a number of interdisciplinary research areas such as biophysics, biochemistry, surface physics, and soft matter physics. The society offers short courses and workshops on crystallography, invites lecturers from abroad, and is very effective at creating new interests and encouraging new students to join this field of knowledge.



1974: A. Guinier, teaching a class at a course on 'X-ray diffraction from imperfect solids' at the Physics Institute, USP – Sao Carlos.

Brazil is affiliated to the IUCr, and the members of the National Committee are appointed by the SBCr. The present members are: G. Oliva (President), I. L. Torriani (Secretary), J. Lima da Silva, A. F. Craievich, and H. Tolentino.



1983: Some of the lecturers at the International School on teaching Crystallography for Materials Science, University of Campinas (IUCr sponsored event). Paul Schmidt, Harry Brumberger, Weinstein, S. Stephens, I. Torriani.

The total number of members in the SBCr is currently 170. The membership includes scientists from other Latin American countries. There are no special interest groups, since the community is not yet organized to that point, but the different labs have a certain specific dedication, and this creates some kind of 'natural' division in the crystallographic interests of the national membership.



Participants of the XVI Meeting of the Brazilian Crystallographic Association – SBCr

What does the SBCr offers to its members? One meeting is organized every two years. A listing of members is updated periodically. Sponsorship is given to courses and workshops in areas related to crystallography. It is difficult to find members that will dedicate much of their time to run the Society, but fortunately there has always been a group that would undertake the task, aware of the fact that there is a lot to be done for the crystallographic community in Brazil.

The SBCr can be accessed from a link through LNLS (www.lnls.br).

2003 Officers of the SBCr

President: Y. Mascarenhas

Vice President: A. Craievich

General Secretary: C. Lariucci

Secretary: R. Itri

Treasurer: M. Fantini

Sec. Teaching Affairs: C. Paiva

Council Members: I. L. Torriani, C. Cusatis, M. T. do Prado Gambardella, G. Oliva, C. A. de Simone, C. Lariucci, N. Speziali, I. Vencato, D. Atencio.

MEETING REPORT

XVI Meeting of the SBCr

March 16-19, 2003

Prof. Richard Garrat (IFSC-USP) showing his 3D models for protein structures.

More than 100 members of the Sociedade Brasileira de Cristalografia (SBCr) gathered in March 2003, at the Physics Inst. of the São Carlos campus of the U. of São Paulo. This was the 16th Meeting since the Society was founded in 1972. Organized every two years, this meeting offers the opportunity for all Brazilian crystallography groups to get together and present their latest achievements. It is also a great opportunity for students, who get a chance to explore the different aspects of crystallography that are active research areas in Brazil.

The meeting was preceded by a two-day workshop on 'Data collection and data treatment strategies using area detectors'. The workshop program organizer and main lecturer, Z. Dauter (Brookhaven), discussed 'Data collection strategies', 'International tables made clear' and 'Index, integration and scaling of data'. His enthusiasm was such that he was also involved in the hands-on sessions in the afternoon, with the collaboration of I. Polikarpov, E. Castellano, J. Ellena and J.R. Sabino, from the IF-SC/USP. A group of twelve students attended this workshop.

The opening lecture on 'Ion gating and selectivity in Gramicidin A' was delivered by W. Duax, IUCr President. This was the first time a high ranking official of the IUCr attended a meeting of a crystallographic society in Latin America.

Oral and poster sessions included 75 presentations on biomolecules, thin films, small molecules, diffraction theory, methods and instrumentation, powder diffraction, crystallographic teaching, and synchrotron radiation applications.

The general subject of structural biology and 'Drug Design in Tropical Diseases' was presented by G. Oliva (U. de São Paulo).

Z. Dauter gave details of the importance of data accuracy in the case of single wavelength anomalous phasing.

Invited lectures on biomolecular crystallography included results on the crystal structure and catalytic mechanism of cellobiohydrolase CelS, the major enzymatic component of the clostridium thermocellum

cellulosome, by B. Gomes Guimarães (Nac'l de Luz Síncrotron) and a new experimental charge density study of Cu(II)-L-alanyl-L-valine by Synchrotron Radiation at 17K by J.R. Sabino (IFSC-USP). M.C. Nonato, (U. of São Paulo) presented a new projet on the rational design of DHODH inhibitors and its applications on the treatment of Chagas disease. J. Lima da Silva, (CNRMN / UFRJ) presented a very interesting and instructive lecture on 'Dynamics and Structure of Macromolecules Involved in Human Diseases'.

On the subject of aperiodic crystals, N. Speziali, (UFMG) presented results on phase transitions and modulated phases in AA'BX₄ Compounds. On subjects more related to materials science, K. Damouche (UNESP) showed the potential use of small angle X-ray scattering in the study of hybrid materials with technological application and F. Rizzo, (Catholic U.), talked about the use of a novel X-ray imaging technique in the study of phase transformations.

Other interesting highlights among the rest of the presentations were:

R. Garrat (IF-SC/USP) showing his injection molded plastic components kits for building 3D molecular models of protein structures and

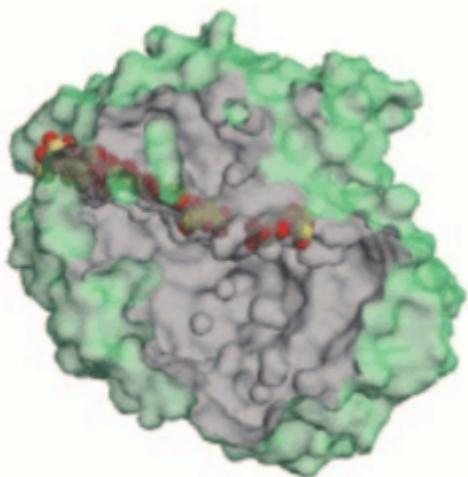
The viability study for the installation of a SANS Beamline at the reactor of the Inst. Nac'l de Pesquisas Energéticas e Nucleares in São Paulo (IPEN-SP)

Two presentations were selected for a more detailed description (see below).

The meeting was sponsored by three Brazilian funding agencies (FAPESP, CNPq and CAPES) and two commercial companies Dairix-RIGAKU and Bruker AXS. The Organizing Committee included Y. P. Mascarenhas (SBCr President, IFSC/USP), N. Speziali (ICEX/UFMG), R. Itri (Inst de Física/USP), I. Torriani (SBCr Council Member, IFGW/UNICAMP), C. Cusatis (Inst. de Física/UFPr), V. Mastelaro (SBCr Secretary, IFSC/USP), C. Lariucci (SBCr Council Member, Inst. De Física/UFG), and F. Rizzo (PUC-Rio).

The crystal structure and catalytic mechanism of cellobiohydrolase CelS, the major enzymatic component of the *Clostridium thermocellum* cellulosome

**B. G. Guimarães^{1#}, H. Souchon¹, B. L. Lytle², J. H. D. Wu² & P. M. Alzari¹,
¹Unité de Biochimie Structurale, Institut Pasteur, Paris, France, ²Dept of Chemical Engineering, U. of Rochester, Rochester, NY, [#]Present address: Ctr de Biologia Molecular Estrutural, Lab Nac'l de Luz Síncrotron, Campinas, SP, Brazil**



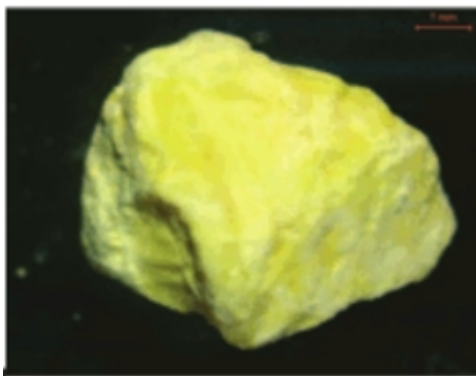
Cut-through of the molecular surface of CelS showing the substrate-binding tunnel with a bound cellohexaose molecule and the open cleft with a bound cellobiose molecule.

Cellobiohydrolase CelS plays an important role in the cellulosome, an active cellulase system produced by the thermophilic anaerobe *Clostridium thermocellum*. The structures of the catalytic domain of CelS in complex with substrate (cellohexaose) and product (cellobiose) were determined at 2.5 and 2.4 Å, respectively. The protein folds into an $(\alpha/\alpha)_6$ barrel with a tunnel-shaped substrate-binding region. The conformation of the loops defining the tunnel is intrinsically stable in the absence of substrate, suggesting a model to account for the processive mode of action of family 48 cellobiohydrolases. Structural comparisons with other $(\alpha/\alpha)_6$ barrel glycosidases indicate that CelS and endoglucanase CelA, a sequence-unrelated family 8 glycosidase with a groove shaped substrate-binding region, use the same catalytic machinery to hydrolyze the glycosidic linkage. The nearly identical arrangement of substrate and functionally important residues in the two active sites strongly suggests an evolutionary relationship between the cellobiohydrolase and endoglucanase families.

Guimarães, B. G., Souchon, H., David-Wu, J. H. & Alzari, P. M. (2002). *J. Mol. Biol.* **320**, 587-96.

Crystal structure of a Th-rich weeksite group mineral.

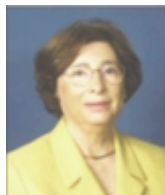
F. M. S.Carvalho, D. Atencio and M. B. Andrade, Dept. de Mineralogia e Geotectônica, Inst. de Geociências,U. de São Paulo



Weeksite is a tectosilicate characterized by a Si:U ratio of 5:2, with chemical formula $\text{Th}_{0.5}(\text{UO}_2)_2\text{Si}_5\text{O}_{13} \cdot 3\text{H}_2\text{O}$. This mineral is found with a number of compositional variations. Th-rich weeksite group specimens from Minas Gerais, Brazil, not yet described in the literature, were studied by X-ray powder diffraction. The possible structural sites occupied by Th were investigated on the basis of WDS chemical analysis and Fourier difference maps.

MISCELLANY

Iris L. Torriani



Iris L. Torriani was born in Buenos Aires, Argentina, and studied physics at the Universities of Buenos Aires and of La Plata. She obtained her undergraduate degree at the latter institution in 1965. Subsequently she became interested in crystallography and joined a group at the Atomic Energy Commission in Buenos Aires dedicated to the study of small organic molecules. In 1967 she was awarded a Fulbright travel grant to pursue graduate studies at the U. of Pennsylvania, Philadelphia, USA. In 1971 she worked on NMR and low-angle X-ray diffraction from model membranes at the Biophysics Dept (Johnson Foundation) of that institution. Upon returning to Argentina she obtained her doctoral degree in physics at the U. of La Plata in 1975. In 1976 she joined the Dept of Condensed Matter Physics at the U. of Campinas (UNICAMP), in Brazil, where her research has been mainly focused on structural problems in solid state physics. Currently she is Associate Professor of Physics and Director of the Applied X-Ray Crystallography Group. Since 1986, she has also been a collaborator at the Brazilian Nat'l Synchrotron Lab (LNLS), where she holds a joint appointment as a research member and coordinator of the small-angle scattering beamline built under her supervision. Her main fields of interest are the application of X-ray diffraction and small-angle scattering to the study of polycrystalline materials, polymers and soft matter, as well as biological macromolecules in solution. She has published 93 articles in international journals and congress proceedings, and directed 8 PhD theses and 15 MSc dissertations.

Since 1989, Dr. Torriani has been Regional Editor for Latin American entries in the World Directory of Crystallographers (IUCr), and since 1999 has been a member of the IUCr Small-Angle Scattering Commission. At the 2003 Congress in Geneva she was elected to the Executive Committee of the IUCr. She is also a Member of the Brazilian Nat'l Council for Crystallography and of the Council of the Brazilian Crystallographic Assn, on which she has served as Secretary, General Secretary, Vice President and President. Other scientific societies to which she is affiliated include the American Crystallographic Assn, the Brazilian Physical Society, the Brazilian Biophysical Society, and the Brazilian Polymers Assn. Dr. Torriani is also a researcher of the Brazilian Nat'l Research Council (CNPq) and referee for several funding agencies in Brazil, such as the CNPq, the Board for Higher Education Programs (CAPES) and the Research Foundation of the State of São Paulo (FAPESP). At the U. of Campinas she is a member of the Selection Committee for Undergraduate Scholarships in the Exact Sciences (CNPq)/UNICAMP and has been appointed coordinator of the Brazil-Argentina Physics Graduate Students Research Program (CAPES/UNICAMP).

MEETING REPORT

Braggs, chemistry and Leeds



Left to right: Charles Bragg, Alison Lowe, David Giachardi, Lady Heath, and Derry Jones

Vacation collaboration in a shed at Leeds U., 1912-1914, contributed appreciably to the science meriting the Nobel Prize for W.H. and W.L. Bragg in 1915. Although the prize was in Physics, X-ray crystal structure analysis has, of course, influenced sciences from mineralogy to medicine. On July 1, 2003, the UK Royal Soc. of Chemistry (RSC) recognized the contribution to chemistry of the Braggs' achievement by making the Leeds site a National Historic Chemical Landmark. WLB's daughter, Margaret (Lady Heath) recalled WLB anecdotes and unveiled a plaque in the presence of the chemist's grandson, Charles Bragg, and of the University's Vice Chancellor (but not the Chancellor, who is unrelated, Melvin Bragg).



D. Giachardi and DWJ Cruickshank

Durward Cruickshank, whose crystallographic career began under E.G. Cox at Leeds (1946-1962), gave a fascinating survey of the 1912-1914 researches and their continuing influence on chemical sciences. Pouring salt and sugar, he noted the long interval between their structure determinations and marveled that WLB, who had determined the NaCl structure in 1913, could draw the lysozyme structure by his 75th birthday in 1965. Durward highlighted how, by the summer of 1912, WHB (1862-1942) and WLB (1890-1970) were well prepared to respond to the discovery of X-ray diffraction by Friedrich Knipping and von Laue. WHB, a mathematician turned physicist, without research training *per se*, began original research (contrast demonstration and confirmatory experiments) in radioactivity in Australia only at the age of 42. By the time he was Physics Professor at Leeds, he was experienced in instrumental manipulation and experimental design and was well-versed in X-ray tubes and the ionization chamber. WLB, a graduate of both Adelaide and Cambridge by age 22, knew the work of W. Barlow on symmetry and the chemist W.J. Pope on how crystals might be structured internally. No doubt this helped him devise the simplifying concept of X-ray reflection in 1912. Father and son then worked ferociously 1913-1914 to determine crystal structures with the ionization spectrometer.

Leeds also figured in the subsequent careers of three of WHB's 1920s collaborators at London's Royal Institution: W.T. Astbury, Kathleen (then Yardley) Lonsdale (who spent 1927-1929 at Leeds), and E.G. Cox. Mature crystallographers will know that Gordon Cox assembled (1945-1957) at Leeds a famous chemical crystallography group whose faculty included George Jeffrey (before Pittsburgh), Durward Cruickshank, Mary Truter, Peter Wheatley, Norman Hartshorne (microscopy), Geoffrey Pringle, and John Robertson. Maturer crystallographers still may recall that in 1946 Leeds had four X-ray groups under: Cox in Chemistry; G.W. Brindley (clay minerals, previously with WLB at Manchester, later at Penn. State) in Physics; W.T. Astbury on wool proteins in Biomolecular Structure; and H.J. Woods on fibres in Textile Physics.

Durward's masterly survey helped chemists celebrate Leeds University's greatest achievement and the youngest Nobel Laureate.

Derry W. Jones

AWARDS AND PRIZES

Another Nobel Prize involving crystallography



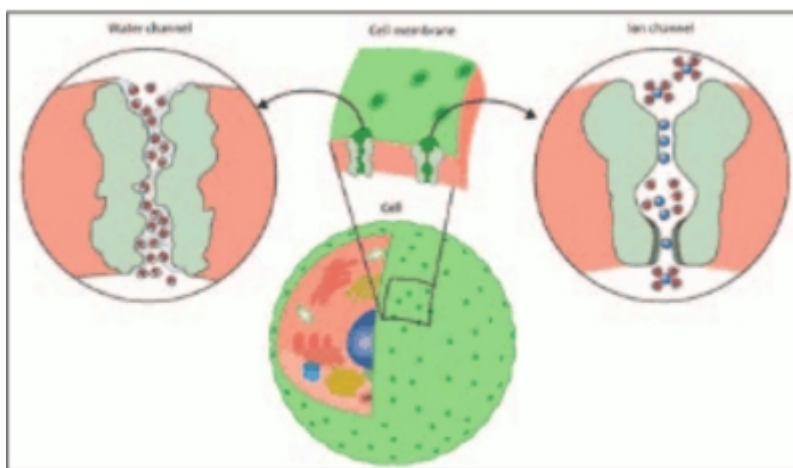
Roderick MacKinnon



Peter Agre

Two Americans won the 2003 Nobel chemistry prize recently for studies of tiny molecular channels in cells that could lead to better treatment of disorders of muscles, including the heart, and other ailments.

The prize went to Roderick MacKinnon, a biophysicist at The Rockefeller U. in Manhattan, and Peter Agre a professor of biological chemistry and medicine at Johns Hopkins U. in Baltimore.



The dividing wall between the cell and the outside world – including other cells – is far from being an impervious shell. On the contrary, it is perforated by various channels. Many of these are specially adapted to one specific ion or molecule and do not permit any other type to pass. To the left we see a water channel and to the right an ion channel.

The two were honored for studies of in membrane channels that transport water molecules and ions. The work opens the door to further research on disorders in which the channels fail to operate properly, including diseases of the nervous system and muscles including the heart.

The image and photo of Dr. Agre were taken from www.hopkinsmedicine.org/press/2003/October/031008A.htm, the photo of Dr. MacKinnon was taken from the website www.rockefeller.edu/pubinfo/profilemackinnon.html

NOTICE

Wave: 1 Duax: 0



On April 24, IUCr President, Bill Duax, was standing on a boulder on the edge of a beach in British Virgin Gorda, when a wave washed over the boulder and threw him 6 ft to the surface of another boulder, breaking his leg. Six ambulances, one ferry boat, two airplanes (including a saber jet), 4 different sets of traction apparatus, 150 medical personnel, and 36 hours later he was in Buffalo where an orthopedic surgeon put his leg back together with a 12 inch titanium plate and 13 screws. Two months later he began walking with the aid of a cane. We hope that by 2004 he will have discarded the cane.

AWARDS AND PRIZES

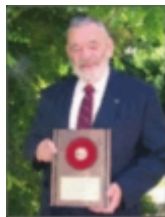
New Fellows of the Royal Society



Three BCA members have been made Fellows of the Royal Society this year. They are **Eleanor Dodson**, Research Fellow at York, **Richard Nelves**, Physical Crystallography at Edinburgh, and **Venkatraman Ramakrishnan**, MRC Lab of Molecular Biology, Cambridge. Full citations may be found on the Royal Soc. website: www.royalsoc.ac.uk/.

AWARDS AND PRIZES

ICDD elects Fellow



William Frank McClune has been elected to the the Int'l Centre for Diffraction Data list of Distinguished Fellows. He is being recognized for his sustained, outstanding work in the field of powder diffraction and was formally honored at the 2003 Denver X-ray Conference.

He celebrates 34 years of service with the ICDD, the past 20 as Editor-in-Chief of the Powder Diffraction File (PDF), nurturing the transition of the PDF from cards and books into the PDF-4 family of relational database products available on CD-ROM and DVD.

Helen M. McDonnell, ICDD

NOTICE

US visa problems

The International Visitors Office (IVO) of the US National Academies has launched a new website to provide information on visas for visiting scientists and scholars and advice for organizers of international scientific meetings in the US. Please see www.nationalacademies.org/visas.

This site includes a questionnaire through which scientists, engineers, medical professionals, and scholars can report their difficulties with the visa process. The questionnaire is used by the IVO to collect statistical data, and, in some cases, to assist with the visa process. The IVO maintains a list of international scientific meetings held in the US. It shares this list with the Department of State on a regular basis to help validate a visa applicant's purpose for visiting the US.

Please visit this site and share it with your colleagues. If you have any comments on how the IVO site can better inform and assist you and your colleagues on visa issues, send them to visas@nas.edu.