

This talk was given by Prof. Gautam R. Desiraju, President, International Union of Crystallography, to the General Assembly of the Union in Montreal, Canada, in August 2014

SLIDE ONE

On behalf of the Executive Committee, I would like to welcome you to the first General Assembly session of the 23rd Congress of the International Union of Crystallography. I would like to thank all the delegates for attending this session and taking part in the General Assembly. I would also like to thank the Local Organisers for the smooth way in which the Congress has been run so far and for making the arrangements for the General Assembly meetings.

SLIDE TWO

Tonight I will give a short introduction to the work of the Union in the last triennium. I will focus on the Union's publications, the International Year of Crystallography and the other activities of the Union. This triennium has seen a great deal of activity and change that will affect the Union in coming years.

In the slide you can see a picture of Abbey Square, Chester, which is where the Union has its offices. Here I have worked closely with the staff to drive forward many of the decisions made by the Executive and Finance Committees.

The Chester office and particularly its publishing operation remains pivotal to the Union. The IUCr is the only scientific Union in ICSU with a significant publishing operation. Revenue from publications provides 93.5% of the income of the Union and makes possible all of the Union's activities.

For several reasons, the Executive Committee has deemed it prudent to increase income from other sources so that revenue from publications does not exceed 80% of the total income of the Union. This would decrease the pressure somewhat on the journals. But this means that we need to identify alternative sources of income.

SLIDE THREE

I would like to take a quick look at the overall financial position of the Union for the last six years. The total cash flow shown on the slide includes all income derived from various sources such as membership subscription, journal and book sales, investment income and bank interest, royalties and advertising income.

The total expenses include all expenses such as journal publication, editorial and technical editing, publication costs of books, journals, and newsletters, and general and office expenses connected with the general secretary and treasurer, and executive secretary.

The net cash flow is the excess of income over expenses for the respective years from 2009 to 2013. You will notice for 2013 for the first time in nearly a decade that we are losing money and we need to be as vigilant as possible to handle this situation in the best way we can. In brief, we need to actively explore all ways of increasing our income and reducing our expenditure.

The Union did not have an investment advisor for five years between 2006 and 2011. In 2011, the Executive Committee appointed Prof. S. Narasinga Rao of the University of Oklahoma as the investment adviser. Prof. Rao has made several imaginative investments for the Union, and these have already resulted in good monetary gains that have been re-invested. Our capital is invested in the U.S. A. and in the U. K. I am indebted to Prof. Rao for scrutinizing our accounts carefully and examining the cash flow, details of which I have just presented.

SLIDE FOUR

As the publishing operation of the Union is so influential, it is all the more important we maintain a competitive position in the publishing arena.

SLIDE FIVE

Over the past decade, funding bodies in many countries have changed the way they fund research and, I think it is fair to say, have become much more analytical in the way they want to see the outcome of research investment. In many countries there has also been a focus on making publicly funded research freely available to the public.

The above developments have led to a number of changes in the publishing world, and here I will highlight two that affect our operations:

Firstly, much more emphasis is now given, rightly or wrongly, to metrics such as h-index and journal impact factors, and this has been something that the IUCr has needed to be aware of in developing our publishing activities.

I do not want to get into an elaborate discussion of h-index and impact factors. They are here to stay, and we need to evolve our journal policies keeping these realities in mind. There is no room for lofty idealism today. The mind, or should I say the wallet, must rule the heart.

Secondly, the last decade has seen the rise of open access in its many forms. The Union has been a pioneer in this area and has seen this as a chance to make the research work published in the journals more easily available to researchers worldwide, through full and hybrid open-access options. The downside has been a fall in subscription revenues and an increase in uncertainty about the future of subscription publishing. Here again, the Union is hedging its bets for a future that is not really predictable.

Additionally, research has become more digital both in the way it is carried out and consumed. The Union's response in this case has been to develop

tools for authors that aid the publication process, and also to move to online only publication of the journals from 2014. The future will only see an increase in developments in this and related fields.

Another development to note is the excellent research now being carried out in regions which historically had not seen any significant research outputs. IUCr publications need to capture this research. The world as they say is flat and we need to shed any kind of fortress mentality in our dealing with various diverse parts of the world.

Finally, we are seeing research breaking down more and more subject barriers. Now routinely chemists, biologists and physicists are joining forces to tackle global research problems and with this shift in work patterns also comes a change in the format researchers want content, how they search for it and ultimately how they digest it.

Crystallography is intrinsically a cross-discipline activity. It is a subject that brings other subjects together. We should be prepared to embrace this reality enthusiastically.

SLIDE SIX

Key developments during the last triennium are a direct result of the business landscape mentioned earlier. To ensure continuity, various changes and appointments have been made which highlight the importance the IUCr places in maintaining and improving its position as an international Union for the crystallographic community.

As such, the triennium has seen some fundamental changes to the journals. At its meeting during the Madrid Congress in 2011, the IUCr Executive Committee set up a Journals Review Committee to consider the medium- and long-term development of the journals. The Committee was chaired by Sven Lidin and reported in early 2012. The journals started the triennium with Gernot Kostorz as Editor-in-Chief who stepped down in 2012. Samar Hasnain was appointed editor-in-chief in August 2012.

At the Adelaide meeting of the Executive Committee in late 2012, the panel approved the establishment of a Journals Management Board (JMB).

SLIDE SEVEN

The journal management board, is comprised of The Editor-in-Chief (chair), the IUCr President, a Main or Section Editor representing each IUCr journal, the Managing Editor, a representative from the IUCr Executive Committee and a representative from the IUCr Finance Committee.

The Journal Management Board is responsible for the management of the publication business of the IUCr including planning and implementation of short-, medium- and long-term objectives for the current and future IUCr journals. The board also has the responsibility for:

- (1) Increasing the influence of IUCr journals among the wider scientific communities covering activities and interest of all of its Commissions
- (2) Broadening the scope of the journals so that high-quality science papers that use crystallography are attracted to the IUCr journals
- (3) Improving the visibility of IUCr journals in non-crystallographic conferences
- (4) Ensuring that emerging fields that use crystallography are evaluated rigorously and captured if appropriate for long-term sustainability and prominence of IUCr Journals

The journal management board considered a detailed plan for journals development. The plan was further enhanced with input from all the IUCr Commissions, broad scientific communities that participate in the Congresses and General Assemblies, and presented to the Executive Committee during its meeting in Adelaide. The Executive Committee approved the development plan for the journals at that time, including the launch of a comprehensive open-access journal in January 2014 bearing the name of the IUCr, simply called IUCrJ. Appointments of ten Main Editors were also approved signaling major changes that were to come in the remaining part of the triennium.

The current slide shows a recent meeting of the journal management board in Chester.

Topics covered during the meeting included

- Widening the scope of the journals so they become relevant to a wider audience
- New Co-editor appointments
- Article publicity and better publicity for author tools
- Business development
- Co-editor meetings in Montreal
- New mechanisms for early decisions on articles
- IYCr2014

The next face-to-face meeting will be May 2015 in Chester

SLIDE EIGHT

The International Year of Crystallography saw the bold step in a bid to rebrand IUCr publications as a key contender in the crystallographic community with the launch of its second truly open access journal simply called IUCrJ. The international year has been an ideal launch pad for the journal. Interest has been high, and at the recent Journal Management Board meeting in Chester editors agreed feedback on the strength of the first issues has been very positive.

SLIDE NINE

The International Year also witnessed the launch of all IUCr journals as online only publications. This signifies a significant change in how we interact with our audience. The digital age is truly upon us and our understanding of how our authors and readers work in the digital space will

govern how we improve our offering over the coming years to meet the needs of the community.

SLIDE TEN

Driving all of these changes has to be the health and well being of the Union and how it serves its committees, key stakeholders, authors, editors and readers. In this slide you can see a graph of the actual number of subscribers to the journals. The number of subscribers has decreased by 3-5% per annum over the last 20 years, based on funding issues mainly. However, from 2004, when the IUCr started to take part in consortial deals, the number of libraries that can access the journals has increased substantially, as libraries that have taken out a Wiley consortial deal can now access the journals. These changes are global and a problem faced by all major publishing houses. Improving the quality of our journals and increasing the spread of communities engaging with our content will steady the attrition giving the Union valuable opportunity to engage with a new and dynamic community and understand in more depth how the growing community wish to engage with us.

SLIDE ELEVEN

The policy of the IUCr Finance Committee has been to try to ensure that the journals make a small surplus for use by the Union for good causes (e.g. support for meetings, workshops, schools, and educational exchange). The slide shows that this has largely been achieved in recent years. However, it is difficult to predict how subscription income will hold up, even in the medium term. To mitigate any uncertainty in journal revenues the Union is considering a number of new business development opportunities, which do include areas such as open access and broader journal development opportunities, but also more longer term opportunities in areas such as membership, events and education.

Taking each of the journals in turn, I will now share with you some of the most important developments on each title.

SLIDE TWELVE

Acta Crystallographica Section A has changed its subtitle to Foundations and Advances.

Advances papers are specially selected papers of higher impact and broader interest. These papers are fast-tracked through the production process and published within 6-8 weeks. Advances will further receive additional publicity to promote the paper through media channels and social networks. Recent special issues include the Bragg centennial issue by Steve Wilkins, and the Laue Centennial issue by Wolfgang Schmahl and Walter Steurer.

At the recent journal management board it was agreed that additional special issues would be commissioned with a view to publishing at least one or two in 2015.

I would like to take this opportunity to remember the tragic passing of Steve Wilkins, an enduring and endearing figure in the crystallographic community. He died while doing what he loved best, teaching a new generation of students at Monash University the science of X-rays. Steve exemplified the quiet achiever and was able to overcome considerable hurdles in seeking the goals he set his mind on. I know I speak for everyone when I say he will be sadly missed.

SLIDE THIRTEEN

Acta Crystallographica Section B sub-title has changed to Structural Science, crystal engineering and materials. To extend the aims and scope of the journal, a new category of paper called Research Perspectives has been agreed which will allow authors the opportunity to see highly deserving papers enjoy the highest status possible for the journal. Marc De Boissieu secured the winners of the 10th Ewald prize as the first Research Perspective.

The first in a number of special issues, Crystal Engineering by Andrew Bond has been extremely successful; I congratulate Professor Bond in bringing out this timely issue which is on par with special issues in competitor journals, in this very fast moving and competitive field. The second special issue is on non-ambient crystallography by Andrzej Katrusiak and is proving equally popular. Due to the success of these special issues, further special issues are in the pipeline; these will cover topics of energy materials and crystal structure prediction.

SLIDE FOURTEEN

Acta Crystallographica Section C has a new subtitle, Structural Chemistry which reflects its new aims and scope. The new subtitle it is hoped will appeal to a more traditional chemistry based audience. The marketing campaign will include promotion of the four special issues already published which will help to endorse the title change and encourage chemists to publish their research in the journal again.

The five special issues on scorpionates, pharmaceuticals, drug discovery and natural products, spectroscopy and theoretical methods for solving chemical problems, and computational materials discovery, have already published and have been well received.

SLIDE FIFTEEN

Acta Crystallographica Section D with an Impact Factor of 7.23 remains the union's highest impact journal. New editors Soichi Wakatsuki and Randy Read have been appointed as new editors.

Methods papers are the most highly cited papers in the journal and a strategy is underway to ensure a pipeline of these papers in the future potentially protecting the journal against fluctuating impact scores year on year. CCP4 special issues have been very successful in the past and this arrangement with CCP4 will continue for the foreseeable future.

SLIDE SIXTEEN

Acta Crystallographica E lost its impact factor in 2013, this was a very serious setback that impinged severely on the Unions finances. A development plan is in place to gain relisting as soon as possible. A new type of paper has been launched called research communications which will sit alongside the current data reports. Research communications are longer articles reporting one or more structure determinations with a full discussion of the key scientific findings. Data reports will be essentially extended abstracts, each describing structures of inorganic, metal-organic or organic compounds. The current subtitle will change in January 2015 to Crystallographic Communications

SLIDE SEVENTEEN

A new type of paper has been launched called research communications which will sit alongside the current data reports. Research communications are longer articles reporting one or more structure determinations with a full discussion of the key scientific findings. Data reports will be essentially extended abstracts, each describing structures of inorganic, metal-organic or organic compounds.

SLIDE EIGHTEEN

Acta Crystallographica Section F has also seen its subtitle change to structural biology communications and as part of the IYCr celebrations a special series entitled crystallisation series has been launched with one paper each issue being published on this theme. The series is proving to be extremely popular and shows all indications of continuing into 2015 and beyond. The Executive Committee in its current meeting has decided to accept an overwhelming opinion within the editorial board of Acta F and do away with the so-called crystallization papers in this journal.

SLIDE NINETEEN

Journal of Applied Crystallography continues to maintain a strong position in the field. The number of papers submitted have doubled over the past 6 years and rejection rates continue to remain steady at around 30%. The current impact factor of 3.34 is dominated by computer programme papers. Plans are therefore being formulated to ensure a steady pipeline of this category of paper to ensure we maintain but importantly improve on our current position.

SLIDE TWENTY

JSR continues to perform strongly; the number of pages and papers are up on this time last year despite no special issues to date in 2014. The hot topic area of XFELs is well covered by the current editorial board and a concerted effort will be made over the coming months to publish more of these papers. Beamline papers are also a high citation source for the journal and plans are currently being laid to increase the number of these papers published in the journal annually. A number of special issues are currently in the pipeline ensuring the journal continues to feature highly in emerging and core markets.

Ilme Schlichting and Friso van der Veen have joined Gene Ice as editors.

SLIDE TWENTY ONE

Ideas for the re-launch of Section B/C/E were discussed by the Executive Committee in August 2013. These ideas were derived from widespread discussions between the section editors and the editor-in-chief that also involved consultation with relevant Commissions and with the working party set up by the editor-in-chief to consider future options for section E. The consensus of the executive committee was that the emphasis of the three journals should be on content, not format.

Clear statements will be publicised which ensure the above message circulates within our communities making the choice of where to publish clear and simple and logical. The message will be communicated through our editors through workshops and drop-ins at conferences and exhibitions, promotional material and editorials and news items posted online.

SLIDE TWENTY TWO

To ensure that the various platforms within the Union function accordingly, a number of key technical developments are currently flagged as critical. These include a major update for the journal web pages, planned to launch this coming autumn, the new web pages will support mobile devices via responsive web design. The new pages will also support closer integration of supporting information adding to the value of our publications. New pre-screening of articles is currently being trialled on a number of journals, with a view to rolling out across all journals if appropriate workflows can be arranged.

New tools to enhance workflows on copyright requests, open access; article processing charges, and general payments are all currently under development.

SLIDE TWENTY THREE

Jonathan Agbenyega took up the position of Business Development Manager in December 2013 to drive through many of the above changes and more.

With an emphasis on new business, other activities will include, OA revenue growth, publicity at a journal and article level, Closer collaboration with commissions and commercial organisations to leverage sponsorship and other collaborative opportunities, closer collaboration with organisations such as CCDC and the PDB and to formulate other strategic alliances

SLIDE TWENTY FOUR

In the last triennium there have been a number of notable developments, these include Carol Brock being appointed editor-in-chief and all eight volumes A to G including A1 being available in print and online.

The International Tables is a flagship product for the Union and as such we will see a substantial effort in repositioning this major reference work

alongside our other publishing activities to ensure we maximise the opportunity of increasing sales and establishing the reference work as a must have publication for best practice and reference within every laboratory carrying out structure determination.

Taking each volume in turn:

Volume A and the Brief Teaching Edition, here work is well under way on new editions. Several new chapters are being worked on and new “general – position” diagrams for the cubic space groups will be included. Publication is due towards the end of 2014.

Volume B, Reciprocal space: The new editor Gervais Chapuis has started work on the fourth edition. Estimated publication date 2016.

Volume C, Mathematical, physical and chemical tables: the new editor Richard Welberry has started work on the fourth edition, again an estimated publication date of 2016.

Volume D, Physical properties of crystals, edited by André Authier, here the second edition went online in 2013, and in print 2014.

Volume F, Crystallography of biological macromolecules, edited by Eddy Arnold, Daniel Himmel and Michael Rossmann, here the second edition went online and in print in 2012.

Volume H, Powder diffraction, edited by Chris Gilmore, Henk Schenk and Jim Kaduk, this new volume is well underway with an expected publication date of early 2015.

Volume I, X-ray absorption spectroscopy, editors Chris Chantler, Federico Boscherini and Bruce Bunker, is currently in development, and finally,

Volume J, (magnetic symmetry) is currently under consideration by the Commission on Magnetic Structures and a decision on this volume will be taken by the Executive Committee in its meeting in Hyderabad in August 2017.

TWENTY FIVE

Moving on to developments associated with the International Year.

TWENTY SIX

In their resolution proclaiming 2014 as the International Year of Crystallography, the United Nations General Assembly recognised that “humankind’s understanding of the material nature of our world is grounded, in particular, in our knowledge of crystallography”.

TWENTY SEVEN

Events taking place throughout the year are truly global in nature and too numerous to mention here in this brief address. However to summarise, events to date have seen the official opening ceremony take place in UNESCO in Paris, where over 800 people attended the two day session. The opening session included a collection of welcome remarks from Ban Ki-moon, the UNESCO Director-General Mme Irena Bokova who formally opened the meeting, followed by welcoming speeches from the President and Vice President of the IUCr, and a representative from the Moroccan government to name but a few. There were speeches from the Nobel Laureate Brian Kobilka, a reminiscence of the last 100 years of crystallography by Jenny Glusker, sessions on crystallography in the BRIC countries, crystallography on Mars and a special highlight on the contributions of young scientists from all over the world.

SLIDE TWENTY EIGHT

The IUCr-UNESCO OpenLabs are in full swing. The OpenLab project has been influenced by the IUCr Initiative in Africa and I will tell you a little more about the initiative in Africa in our next slide. So far we've seen OpenLabs in Pakistan, Argentina, Morocco, Ghana, Cambodia and Uruguay; the next will take place in Turkey this coming September. For those who do not know, the OpenLabs are crystallographic laboratories based in different countries worldwide. Each of them is organized by IUCr, UNESCO, a company or companies, and a local host. IUCr typically designates an instructor or instructors and provides financial assistance. The company provides the experimental facility and the local host organizes the nitty gritty of the meeting. UNESCO augments fund collection through governments. The OpenLabs are aimed at allowing access to crystallographic knowledge and technology, key for the fruitful development of science, and are intended to open possibilities for conducting high-level research

TWENTY NINE

As mentioned in my previous slide the IUCr initiative in Africa was approved in 1999 by the IUCr Executive Committee following a proposal of Jan Boeyens from South Africa. This initiative has been aimed at providing training in crystallography teaching and research methods to faculty members and students from the most disadvantaged parts of the world. Since its launch the IUCr has organised a number of courses, initially in English-speaking African countries in collaboration with the South African Crystallographic Association. Since 2007 our Vice President Claude Lecomte has assumed responsibility for the project. He has worked tirelessly and the initiative in Africa has developed rapidly with activities in Congo, Zimbabwe, Cameroon and Ivory Coast. He has been assisted in these activities by Luc Van Meervelt. These activities have been implemented in collaboration with manufacturers such as Bruker. The IUCr has covered transportation expenses and the recipient university the maintenance expenses. The Union is committed to a continuing and ongoing interaction with Africa.

SLIDE THIRTY

The IUCr-UNESCO summit meetings are intended to bring together scientists from countries in three widely separated parts of the world, using a common crystallographic theme. There is a real necessity for scientists to think beyond political borders and other distinctions. Therefore the summit meetings, which will be attended by scientists in academia and industry, and by science administrators, are planned between countries which have hitherto been divided on the basis of geography, ethnicity, religion and politics. These meetings will focus on high level science, also highlighting the difficulties and problems of conducting competitive scientific research in different parts of the developing world.

THIRTY ONE

The first meeting in Karachi, Pakistan was a great success and saw a historic moment witnessed when over 50 leading scientists from the South and East Asian region, notably China, India and Pakistan, signed a general appeal to the IUCr to help in initiating actions to promote regional scientific collaboration including but not limited to joint holding of training workshops, video-based lecturing, encouraging mobility of researchers, promoting joint research projects and facilitating regional conferences on the subject of X-ray diffraction and its applications in the South Asian and South East Asian regions. For me, as an Indian, it was a special privilege and honour to lead a group of 15 Indian scientists to Pakistan where we were given an enthusiastic and heart-warming reception.

THIRTY TWO

A major objective of the International Year of Crystallography is to establish a vibrant worldwide network of schools participating in crystal-growing experiments nationally and internationally. Many children and countries are already involved including Belgium, France, Spain, Singapore, Canada, England, Australia. The competition will introduce students to the exciting and challenging world of growing crystals. Prizes will be awarded for the best videos or essays describing the crystal growing experiment. Educational material for teachers prepared by the IUCr and the working group for the competition is available.

THIRTY THREE

I cannot end my discussion of the International Year of Crystallography without a very quick mention to the wonderful work of our volunteers out there in the community. Your activities and support are too numerous to mention here, however just as a small example of the enthusiasm and good will the IYCr2014 brochure "Crystallography Matters" has now been translated by volunteers into 15 languages, including French, German, seven Indian languages including Hindi and Urdu, Italian, Thai, Macedonian and Japanese.

THIRTY FOUR

The final part of my talk covers the other activities of the Union

THIRTY FIVE

One of the aims of the International Year has been to increase the number of countries involved in the Union. Currently, the Union has 42 adhering bodies representing 51 countries. A further 11 countries will be putting forward applications for membership during the 23rd General Assembly.

The Executive Committee has considered these applications and is pleased to recommend to the General Assembly that these countries be admitted. The Latin-American Crystallographic Association (LACA) will formally request membership of the Union at a regional level to join other regional associations; the European Crystallographic Association (ECA) which became a member in (1978), the Asian Crystallographic Association (AsCA) which became a member in 1987 and the American Crystallographic Association (ACA) which became a member in 1990. Crystallography in South America is definitely on an upsurge and the Executive Committee feels that the incorporation of LACA as an IUCr Associate is both timely and necessary.

THIRTY SIX

Acting on the recommendations made by the Sub-committee on the Union Calendar, the IUCr have supported over 100 scientific meetings in 34 different countries since 2011. The scope of the meetings that may be supported through the Sub-committee on the Union Calendar has been extended so that national meetings that are held in developing countries are now included.

THIRTY SEVEN

The IUCr Visiting Professor scheme aims to support some of the costs of having internationally recognised scientists as lecturers for short courses at workshops or schools organised in developing countries. These schools or workshops may have national or international character. Up to a maximum of three Visiting Professorships can be granted for a single event. Travel and insurance costs will be met by the IUCr, while the local organisers cover the accommodation and subsistence expenses. Support from at least one IUCr Commission is required. We would give maximum consideration to applications for Visiting Professors to go to South America, Central America, Africa and disadvantaged areas within Europe and Asia.

THIRTY EIGHT

The IUCr has established a bursary scheme for young scientists attending the annual meetings of the Regional Associates. This is additional to the young scientist support that the IUCr already provides and is aimed at facilitating the attendance of young scientists from the area covered by one Regional Associate at a meeting of a different Regional Associate. The aim is to broaden the knowledge of the awardees and enable them to establish contacts that will be of help to them in their careers.

The scheme is run by the IUCr and is the responsibility of the Executive Committee, which has a sub-committee to select successful applicants.

THIRTY NINE

I would like to draw your attention to the IYCr legacy fund. This fund has been established to maintain the momentum of the International Year and carry on activities in general outreach and training beyond IYCr2014. I would urge you to visit the IUCr booth in the exhibition area and to donate generously. Your contribution would be tax deductible.

SLIDE FORTY

During my presentation you have heard a description of a large growth in activity in our publishing programme and throughout the IUCr. This upsurge in activity is due to the rapidly changing landscape of the publishing world and the growing needs of the crystallographic and related scientific communities.

When you consider the scale of these activities, which include the journal rebranding exercise, new submission and validation tools, refreshing the aims and scopes of the journals, and work on improving outreach to new countries and communities, you can begin to understand that we need the help of the whole community in this endeavour.

Without you, in your roles as our authors, editors and, reviewers, and supporters of our journals we would not be able to achieve many of the objectives we have planned. I would like to take this opportunity to thank you all for your continued support and guidance through these developing times.

A tremendous effort has been witnessed during the International Year from volunteers and advocates willing to give their time and experience freely to ensure the year achieves its goals. The list is too long to mention all the individuals by name, I would just like to take this opportunity to thank you one and all for this unstinting support.

I would also like to thank my colleagues on the Executive Committee for their dedicated work for the Union. In addition, I would like to thank all those who have committed their time to the Union in the last triennium. In particular, the more than 240 Editors and Co-editors who have worked on the journals deserve our thanks.

Without the support from this dedicated group we would not realise the successes we have seen in our journals and business as a whole.

Finally a big thank you also goes out to the Chester staff in facilitating and supporting all of these efforts.