

23 - 31 July Montevideo Uruguay





# and other IYCr2014 activities in Uruguay



#### Leopoldo Suescun, Assoc. Prof.

Crystallography, Solid State and Materials Chemistry Laboratory Cátedra de Física/DETEMA Facultad de Química Universidad de la República Montevideo, URUGUAY

IYCr2014 activities coordinator in Uruguay

# Uruguay in Latinamerica



Latin America: 24 countries in 2 continents (North and South america)

Uruguay in Latin America (and the world):

- 11th in land area between Ecuador and Nicaragua (91st)
- 20th in population between Puerto Rico and Guiana (131st)
- 17th in poulation density between Perú and Argentina (197th)
- 3rd in GDP per capita between Argentina and Panama (60th)
- 3rd in human development between Argentina and Cuba (50th)
- 1st in GINI Index ahead of Nicaragua (between Israel & Thailand)
- 2nd in student performance (PISA) between Chile and Mexico (44th)

http://en.wikipedia.org/wiki/Latin\_America http://en.wikipedia.org/wiki/List\_of\_countries\_by\_Human\_Development\_Index http://en.wikipedia.org/wiki/List\_of\_countries\_by\_GDP\_(PPP)\_per\_capita http://en.wikipedia.org/wiki/List\_of\_countries\_by\_income\_equality http://en.wikipedia.org/wiki/List\_of\_countries\_by\_student\_performance

# Grupo de trabajo del Año Internacional de la Cristalografía 2014 de Facultad de Química.





Nicolás Estefan
Mauricio Rodríguez
Natalia Álvarez
Andrés Cárdenas
María Isabel Galain
Miriam Barros
Maia Mombrú
Ivana Aguiar
Guzmán Peinado
Ivana Núñez
Leopoldo Suescun



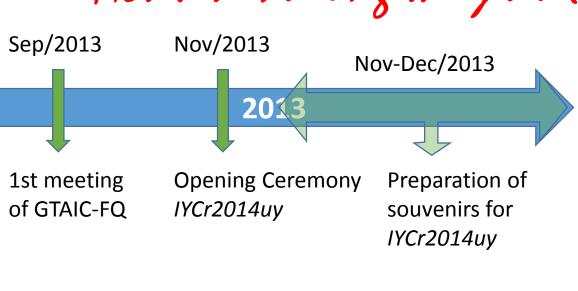
## The 14 Cr 2014 in Uruguay

Concurso de Crecimiento de Cristales nara estudiantes y núblico en general en Uniquay



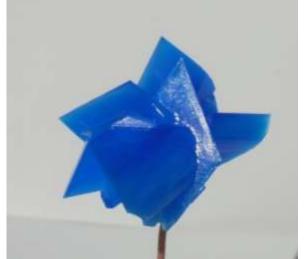
Greece

## Activities along the year (and more)





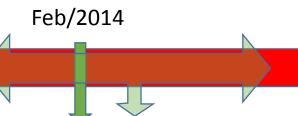






## Activities along the year (and more)

Sep/2013 Nov/2013 Nov-Dec/2013 2013



1st Activate of and Distancias:

IYCr2014 Secondary school
Conference by ers on a monthAlessia Bacche stay in the lab
growing crystals



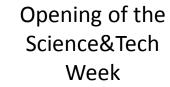




# Activities along the

Sep/2013 Nov/2013

Nov-Dec/2 2013 Feb/2014 May/2014

















May-Aug/2014

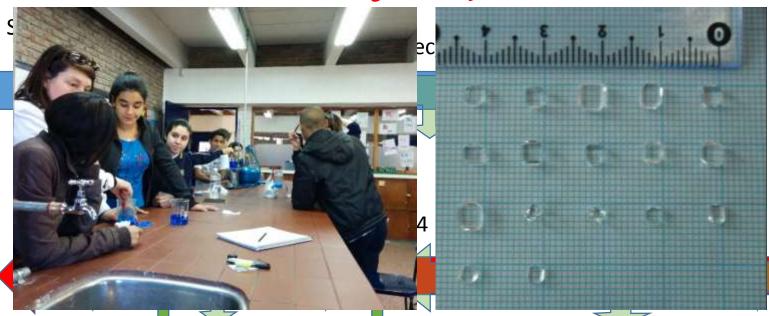




Training tutors for
Crystal Growth Competition
and Talks for Schoolchildren
form 6 to 18 years old and
also adults in night school.
More than 50 talks given by
many members of the
GTAIC-FQ



## Activities along the year (and more)





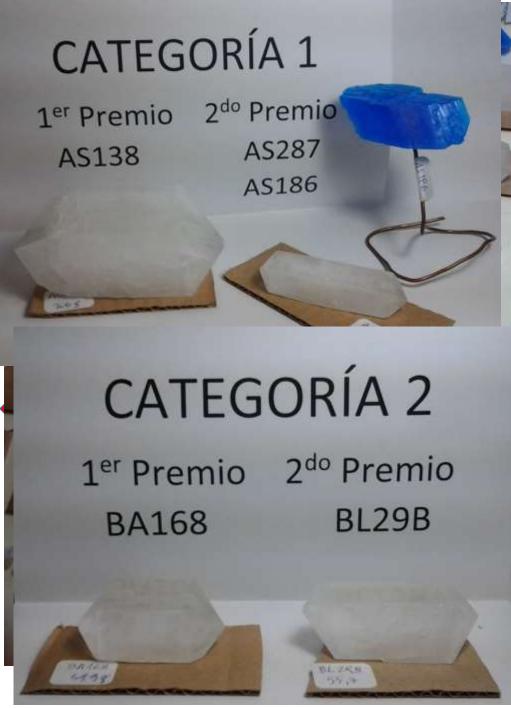
Aug-Sept/2014

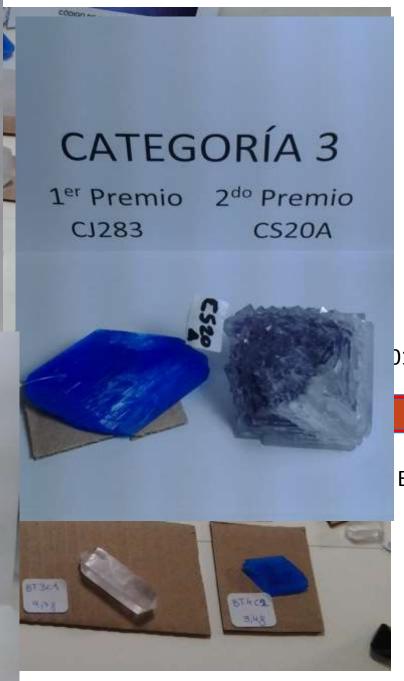


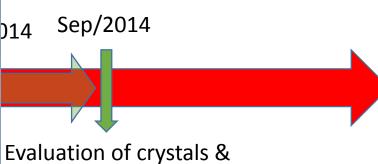


Crystal growth period.









Winners Announced













Public exposition and Prizes given in Closing Ceremony





- July: S crysta
- Septer
- Nover
- Crysta
- Decen











- Preparation & First discussions: June 2013
- Confirmed dates: March 2014
- Pre-registration Opening: March 8th, 2014
- Pre-registration Closed: April 20th, 2014
  - **52 people registered** (undergrad., Master & PhD Students and Young Researchers)
  - 4-Argentina, 6-Brazil, 11-Colombia, 4-Costa Rica, 3-México, 1-Nicaragua, 8-Perú, 12-Uruguay, 3-Outside the región (Canada, Phillippines, Pakistan).
- Final Program: April 23rd, 2014
- Selected participants (20 seats available): April 30th, 2014
- Final list of Lecturers: April 30th, 2014
- Final list of Participants: July 22nd, 2014
  - **20 participants** (12 received transportation, lodging and subsistence support).
  - 4-Argentina, 3-Brazil, 3-Colombia, 1-Costa Rica, 2-Perú, 7-Uruguay





 9-day program going from the history to advanced topics, covering the theory and experiment. A full day plus at least additional 16 h during the 4rd to 8th day devoted to data collection and analysis.

	Wed, July 23		Fri, July 25	Sat, July 26	Sun, July 27	Mon, July 28	Tue, July 29	Wed, July 30	Thu, July 31
8:00-10:00	Registration	Topic 2-Lecture 1. X-ray scattering Bragg's Law & Reciprocal Space	Topic 3-Lecture 1. The phase problem. Intensity equation. Patterson Method	Topic 4-Lecture 1. Structural refinement R and GooF parameters	Data Collection Session	Topic 4-Lecture 3. Crystallographic computing, structural analysis and reporting.	Official Opening Ceremony. Group Photo	Topic 6-Lecture 1. Charge density analysis.	Presentations of results by participants (short presentations)
10:00-10:30	Opening	Coffee Break	Coffee Break	Coffee Break		Coffee Break	Coffee Break	Coffee Break	Coffee Break
10:30-12:30	Brief history of Crystallography and the IYCr2014	Topic 5-Lecture 1. Introduction to S.C. diffractometry. Crystal Mounting	Topic 5-Lecture 2. Cell determination (indexing) and data collection strategy	Topic 5-Lecture 3. Data Integration and Scalling	Data Collection Session	Topic 5-Lecture 4. Space Group determination and Structure Solution	Topic 5-Lecture 5. Structural refinement and final reports.	Topic 5-Lecture 6. Twinning.	OpenLab evaluation and Closing Ceremony
12:30-14:30	Lunch Break	Lunch Break	Lunch Break	Lunch Break		Lunch Break	Lunch Break*	Lunch Break	
14:30-16:30	Topic 1-Lecture 1. International Tables and Space Group symmetry.	Topic 1-Practise 2. Cell transformations	Structure Factor Calculations	Topic 4-Lecture 2. Crystallographic Databases	Data Collection Session	Topic 4-Practise 1. Crystallographic calculations with the metric matrix.	Topic 5-Practise 4. Practise on struct determ w/own data.	Topic 5-Practise 5. Practise on struct refinemen w/own data	
16:30-17:00	Coffee Break	Coffee Break	Coffee Break	Coffee Break		Coffee Break	Coffee Break	Coffee Break	
17:00-19:00	Topic 1-Practise 1.Symmetry 2D&3D Patterns	Topic 2-Lecture 2. The structure Factor	Topic 5-Practise 1. Crystal selection and mounting	Topic 5-Practise 2. Cell reduction and data collection practise	Data Collection Session	Topic 5-Practise 3. Practise on S.G. Symmetry determination	Topic 4-Practise 2. Structural analysis and reporting. Building CIF file.	Topic 5-Practise 6. Building a CIF for Acta E w/own data.	





#### • Budget:

Income:

• IUCr/IYCr OpenLab – Bruker: 10.000 US\$

UNESCO Regional Office for Science in Latin America and the Caribbean:
 3.000 US\$

Ministry of Education of Uruguay (Permanent Commission for UNESCO): 1.500 US\$

• Expenses:

• Transportation (12 Students, 1 Lecturer): 6.365 US\$

• Lodging (12 Students, 2 Lecturers): 3.850 US\$

• Subsistance (13 Students, 2 Lecturers): 2.438 US\$

Organization expenses (course material, coffee breaks, etc.)
 1.986 US\$

- Bruker–designated participants (2 salesman, 1 Lecturer) at no cost for the organization.
- IUCr Vice-President Claude Lecomte joined (local expenses covered by organization).







- Lecturers (and some colleagues):
- Claude Lecomte
- Bruce Noll (Bruker)
- Javier Ellena (IFSC-USP, Brazil)
- Álvaro W. Mombrú (Group Leader)
- Ricardo Faccio
- Leopoldo Suescun
- Prof. Raúl Mariezcurrena (Group Leader from 1973 to 2002)
- Santiago Vázquez (my PhD student)









Inauguration of the OpenLab and the Bruker D8 Venture Diffractometer





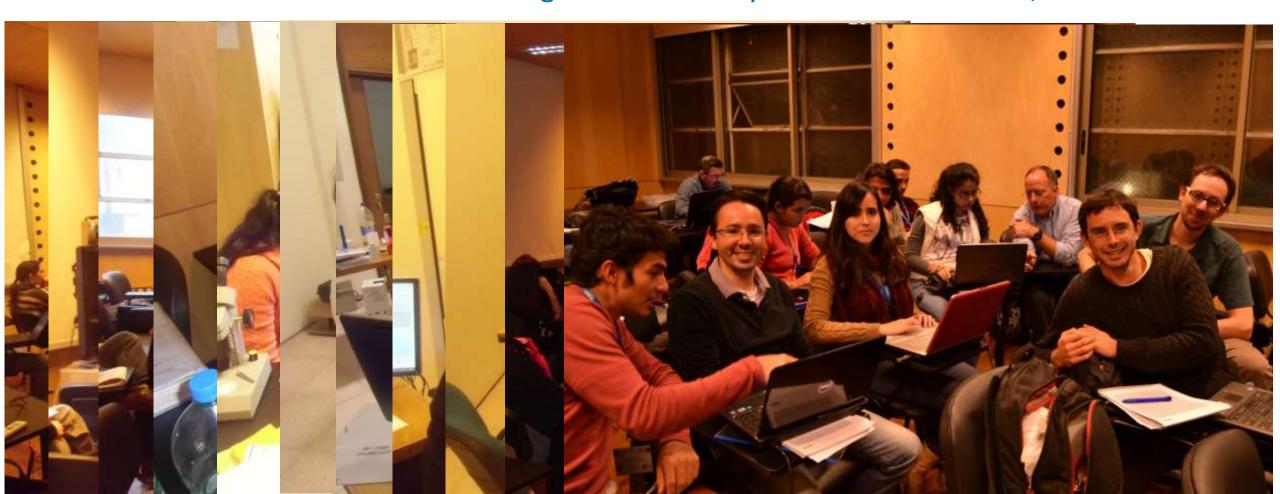
Authorities from Universidad de la República, the School of Chemistry, PEDECIBA, and Funding Agencies (ANII, CSIC) were invited to join the IUCr and Organizers to cellebrate the installation of the new instrument and the OpenLab that was possible after it's purchase.







• Hands on: 13 students that brought their own crystals took home data/results.









• Students:



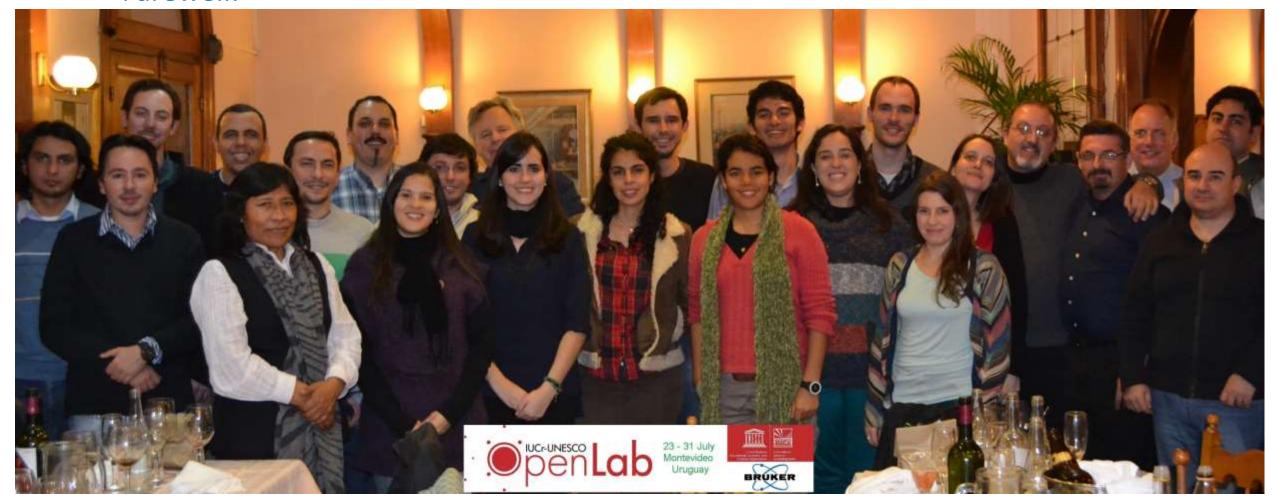


23 - 31 July Montevideo Uruguay





• Farewell:





Innovation with Integrity





Noise was made:





supported OpenLab, in Montevideo, Uruguay. This 9-day school was organized by Leopoldo Suescun (Facultad de Química: Universidad de la República) as part of the glob IYCR activities. The school had a strong focus on singlecrystal X-ray diffraction (SC-XRD) and took advantage from the brand-new DB VENTURE. Beforehand, students were incouraged to bring real examples from their laboratorie

escun, Ricardo Faccio, Alvaro W. Mombru (Universid and En the Moll (En keel provided intensive training cover analysis on the instruments installed at home. Many of th weakly diffracting samples indeed required the intensity of the IuS microfocus X-ray source. All made advantage of the shutterless operation of the PHOTON 100 detector and the most efficient data collection. With skills learned during the workshops, the students were able to analyze and refine th data using APEX2. In the end, students and the faculty left newly impressed about modern instrumentation's possibility and the fascinating science of crystallography

Guzmán P.: "It a very thorough by the Bruker diffrac

Lorena M.: "The course [...] was a very good experience. [...] it was great [to have] the possibility of actually do the whole process of measuring and refining by ourselves, I mean, setting up the whole experiment with our own hands. This wouldn't have been possible without the help and almost infinite patience of Bruce Noll (I take this opportunity to express my gratitude)"

Lisandro O.: "As student of the course I can tell you that the experience was really rewarding. Everything was perfect and one could feel that nothing was done at random. I really enjoyed being part of it. [...] We recently bought a diffractometer D8 QUEST from Bruker and are solving difficult protein structures in-house, that is why we are really happy with the equipment. "

measure their ow installed just one received from Le extremely useful. and always enerc problem whatsoe

### IYCr OpenLab

"I discovered a great new world of possibilities"

www.bruker.com

Crystallography

#### IYCr OpenLab

"I discovered a great new world of possibilities"

Innovation with Integrity

Pressure Workshop

crystallographers

■ ECM28 satellite meeting

ACA 2013

Senior

■ ECM28

Difractometro de Monocristal Bruker D8 Venture instal

Este martes 29 se realizará en la Facultad de Química de l

de un difractómetro de rayos X de monocristal automático o

investigación de primer nível en cristalografia. Será presen

por la Unión Internacional de Cristalografía y la UNESCO o



23 - 31 July Montevideo Uruguay







During the official Opening Ceremony of the OpenLab, the official inauguration of the Single-Crystal X-ray Diffraction Laboratory of

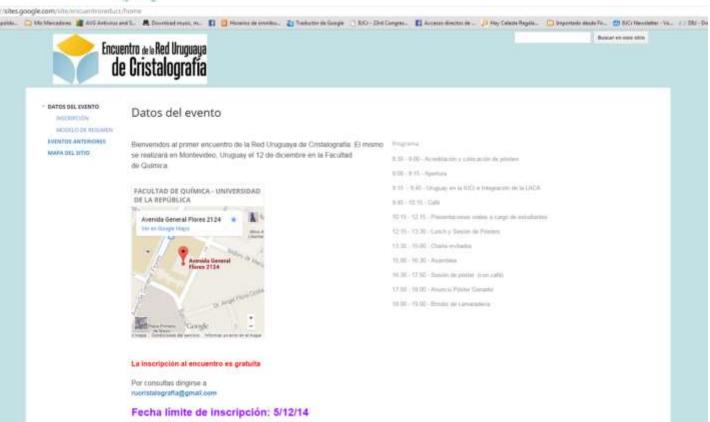
Química, the Comisión Sectorial de Investigación Científica (CSIC), the Agencia Nacional de Investigación e Innovación (ANII) and

the Facultad de Quimica took place, in the presence of authorities or representatives from the U. de la República, the Facultad de

on charge-density analysis given by Claude Lecomte, Vice-President of the IUCr.

- The first National Meeting on Crystallography in Uruguay took place at the Facultad de Química, Universidad de la República, Montevideo on December 12th, 2014 to cellebrate Crystallography and the IYCr2014 in academia.
- 50 registered participants (35 maximum attendance).
- First Assembly of the RUCr decided to organize the second Meeting in 2015 and study the possibility of becoming a formal association or society in 2016.
- A poster prize was given consisting on a plane ticket and 400 US\$ for expenses for the winner to present his work at the Meeting of the LACA next September.







# Encuentro de la Red Uruguaya de Cristalografía







Poster prize for Santiago Vázquez for the work "Síntesis y caracterización de  $La_{0.6}Sr_{0.4}Fe_{0.8}Cu_{0.2}O_{3-\delta}$  como cátodo para celdas de combustible de temperatura intermedia"

# Fun events: Vino Cristalizado



LAS VIOLETAS

#### Cristalizado

Este vino fino Tentat rusado la sido elaborado cordensendo cristalem naturales de artinso ácido de portusa y fine sefeccionado por los profesares de la Seccióo Enologia de la Facultad de Química, Eshanto Bosido y Francisco Carras en colotración del Año Intersaccional de la Cristalogogía 2014.

El Químico Louis Pastour en sus primeros estudios sobre el vinto descobrio en 1848 que el natrato del vino (may utilizado hoy comos sales digueño as) cristalizaba de dos formas distintas que eran imágenes en el espeja una de la otra y ópticamente activas, masmando las diferencias moleculares llamadas, levógiras o destrogira. Este descubrimiento fue uno de los apuntes más significativos de la cristalografía a la quirroca del siglo XIX. Lo celebramos con este vino Tantel, la variedad insigne del vino Uniquaya, conteniendo entatles de tartinto ácido de potusió, el compuesto processor de tan importante hallanga que se otravienne enfranda las botellas hautas su cristalización.

PAIR TOP OF THE CONTROL OF THE CONTR

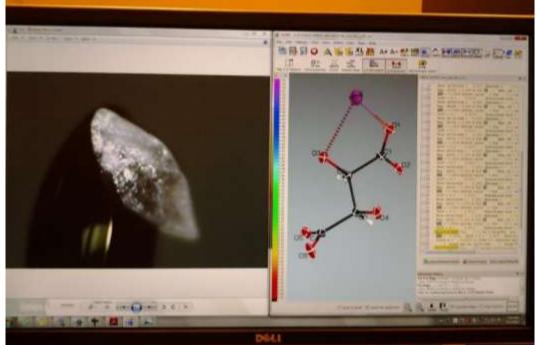
www.cristalografia2014.fq.edu.sq/visus











## Fun events: (Qué es un cristal? video

Video ¿Qué es un cristal?

Video available in YouTube Channel PEDECIBA25

# Acknowledgments

#### **Companies/Organizations**

- Facultad de Química University of Uruguay.
- IUCr
- Bruker
- UNESCO
- Ministry of Education and Culture, Uruguay
- PEDECIBA
- ANII
- CSIC UdelaR
- Museum of Natural History "Carlos Torres de la Llosa"
- ANEP (National Administration of Public Education)
- Companies: DIU, PERRIN, Mercurio Viajes
- Institut Pasteur Montevideo
- TarkioFilm

#### **People**

- All members of GTAIC-FQ specially Guzmán, Nicolás and Natalia. Eduardo Manta (former Dean), María H. Torre (Dean), Alvaro Mombrú and all my coworkers.
- Claude Lecomte, Gautam Desiraju, Michele Zema and all Chester staff.
- LACA mates, especially Diego, Ernesto and Graciela.
- Ernesto Fernández-Polcuch, Soledad Benítez and Paula Santos.
- Andrea Vignolo, Gabriel Antablián, Gustavo Riestral, Leonardo Laborde.
- Gregory Randall and Cecilia Fernández.
- Jacqueline Prochet and Josefina Ordeix.
- Insp. Quim. Mónica Franco.
- Guillermo Sanguinetti.
- Horacio, Daniel, Toty, Daniela.
- Guille Kloetzer, Virginia Chiappe, Rafa, and Virginia Bogliolo

# Special thanks to

### Organizers of the IYCr2014 Legacy Conference

- Abdelmalek Thalal
- Michele Zema
- Claude Lecomte



#### And you for your kind attention

- Questions? Comments?
- Contact me at leopoldo@fq.edu.uy or leopoldosuescun@gmail.com

• Sorry, no more wine available...