

IUCr-UNESCO OpenLab “Resolución de estructuras cristalinas por difracción de rayos X de monocristal”, Montevideo, Uruguay, 23rd – 31st July, 2014 with the support of Bruker.

A Type 1 OpenLab was held in Montevideo, Uruguay this southern winter motivated by the recent installation of the Bruker D8 Venture diffractometer at Facultad de Química, Universidad de la República, Montevideo. The event, organized by the Laboratorio de Cristalografía, Estado Sólido y Materiales (Cryssmat-Lab), Cátedra de Física, DETEMA and supported by Facultad de Química, Ministerio de Educación y Cultura of Uruguay, the Regional Office of Science for Latin America and the Caribbean of UNESCO and the International Union of Crystallography brought together 20 participants (young professors and advanced PhD students) from Argentina, Brazil, Costa Rica, Colombia, Perú and Uruguay that had the chance to learn the fundamentals and applications of single crystal x-ray diffraction. From the 20 participants 13 brought single crystals and were able to collect data and make the structure determination and refinement of their own structures on site and had the chance to follow the whole process from crystal mounting to CIF preparation with their own samples and results.

The OpenLab program included 14 hours of Lectures and 12 hours of Practical sessions on history and fundamentals of crystallography, taught in Spanish, by the Organizers Prof. Leopoldo Suescun, Prof. Álvaro W. Mombrú and Prof. Ricardo Faccio from Facultad de Química, and the invited Professor Javier Ellena from Instituto de Física de Sao Carlos, Universidade de Sao Paulo. Additionally, it included 12 hours of Lectures and 12 hours of Practical sessions on application of single crystal diffractometry taught by Dr. Bruce Noll from Bruker. He also devoted a very significant number of hours helping the participants select and mount their crystals, performing crystal evaluation and data collection setup and guiding the data processing and structure determination process of organic, metal-organic, mineral and metallic samples.



Left: Dr. Bruce Noll lectures the participants on crystal mounting and centering. Right: Participants Geraldine Hernández (Colombia), Andrea Naranjo (Brazil), Martín González (Brazil), Andrea Araya (Costa Rica) and Nilda Pinto (Perú) during a session of crystal selection and mounting in the Lecture room.

One full day of the program (Sunday, July 27th) was devoted to collect data, to allow all participants have their own data to work on practical aspects of refinement and CIF construction by themselves. Finally, the advanced participants very well received a special topic Lecture on charge density analysis given by Prof. Claude Lecomte, vice president of the IUCr.

During the official Opening Ceremony of the OpenLab the official inauguration of the Single Crystal X-ray Diffraction Laboratory of Facultad de Química took place with the presence of authorities or representatives from Universidad de la República, Facultad de Química and Comisión Sectorial de Investigación Científica (CSIC), Agencia Nacional de Investigación e Innovación (ANII) and Programa de Desarrollo de las Ciencias Básicas (PEDECIBA), who provided the funds to purchase the instrument. The vice president of the IUCr, Claude Lecomte, introduced the IYCr2014 to the participants and representatives from UNESCO and the

Ministry of Education and Culture of Uruguay (co-sponsors of the OpenLab with Bruker) emphasizing the importance of the state-of-the-art equipment now available in Uruguay thanks to the synergic work by IUCr, local Uruguayan agencies and Bruker.



Left: Natalia Álvarez (Uruguay), Mario Macias (Colombia) and Javier Ellena (Brazil) follow the refinement of a structure by Olga Sánchez (Argentina) assisted by Bruce Noll (USA). Right: Authorities and representatives from the Funding Agencies and Sponsors of the OpenLab, M. Salgueiro - ANII, A. W. Mombrú - PEDECIBA, E. Fernández Polcuch - UNESCO, G. Aintablián – DICYT-MEC, L. Suescun – Organizer, A. Vignolo – MEC, M. H. Torre Dean of Facultad de Química, C. Lecomte - IUCr Vice President, E. Manta former Dean of F.Q. and L. Franco-Fraguas – PEDECIBA-Q after the cut of the ribbon inaugurating the single crystal x-ray diffraction laboratory of F.Q. in front of the Bruker D8 Venture Diffractometer.



Participants of the IUCr-UNESCO OpenLab of Montevideo, Uruguay.

The last morning of the event was devoted to presentations by the participants. Those who solved their structures showed their results, discussed their problems and received advice on how to finalize their works from other participants and lecturers. The last activity was the evaluation of the event. A round of comments from the participants suggested a unanimous positive view of the event when considered globally. Suggestions on the time distribution and an emphasis on different topics were received and will be used to adjust the program for future events of this kind. The list of participants including contact information and a summary of answers from a detailed and anonymous evaluation questionnaire is available from the web site of the OpenLab (www.cryssmat.fq.edu.uy/OpenLab/evaluationbyparticipants.pdf).

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