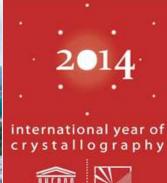


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DEPARTMENT OF CHEMISTRY



Asian small-molecule crystallography school







3-7 December 2014





Organizers:

Local IUCr Representative Prof. Ian WILLIAMS Prof. Michele ZEMA

HKUST, Hong Kong U. Pavia, Italy

Other lecturers:

Dr. Fraser WHITE Agilent Tech., Oxford, U.K.

Dr. Horst PUSCHMANN OlexSys, Durham, U.K.

Dr. Alison EDWARDS ANSTO, Australia

Prof. Birger DITTRICH U. Hamburg, Germany

Small molecule Workshop: Topics

- 1. Crystal Growth Theory and Practice
- 2. Basics of X-ray Diffraction, Crystals and Symmetry
- 3. Structure Determination Overview
- 4. Selecting and Mounting Crystals
- 5. Diffractometer I. Pre-experiment:

Unit cell and Space group determination

- 6. Diffractometer II. Data Collection and Reduction
- 7. Using the OLEX2 Software Package
- 8. Structure Solution and Refinement
- 9. Validation, Tables and Figures
- 10. Databases and Publication
- 11. Neutron diffraction, Problem Structures



Den Lab 3-7 December 2014









Lectures, **Tutorials** & **Presentations** were held over **five days**, giving introductory theory, practical worked examples, an **Olex2** workshop as well as more advanced themes



Dipentab 3-7 December 2014

Practical sessions on single crystal X-ray diffractometry and crystal growth also held





December 2014



A total of **38 participants** were registered with 20 from outside of Hong Kong, including Philippines (6), China (5), Thailand (4), Malaysia (3), India (2) and 18 participants were from 4 universities within **Hong Kong**.



Dipental 3-7 December 2014

Achievements and Legacy:

Hong Kong Open Lab one of several in SE Asia with Rigaku Open Lab in Cambodia (7-11 Jul) and Bruker Open Labs in Indonesia (18-22 Aug) & Vietnam (8-12 Dec)

Training and support of young research-active and upcoming **service crystallographers** (Philippines, Thailand, Malaysia).

Set up of several new collaborations (e.g. U.Philippines-Diliman – HKUST).

Proposal of 1-day crystallographic symposium Manila, Philippines, Spring 2016

New lab initiatives for **training and demonstration** & foundation for 'recurrent' **OpenLabs** around the region.

Initiation of IUCr-sponsored X-ray diffractometer renovation and transfer.