Olex2 Asian Workshop: AsCA'13 Hong Kong,
Saturday 7 December 2013

Olex2 is a very powerful software package to assist with all stages of a crystallographic structure determination from structure solution through refinement to image, report and CIF generation. For beginners this 1-day workshop will give a good introduction to Olex2 highlighting its key operations by working through a complete structure determination process. For existing users in the afternoon we showcase some of its unique advanced tools that are available to assist/ simplify your work as a structural analyst and crystallographer. The workshop will be informal, and there will be plenty of time for hands-on experience with Olex2. Short sets of instructions will be followed by 'now-do-it-yourself' sections during which we will be available to assist (in English and Chinese) and help sort out any problems you may encounter. Please remember to bring your lap-top and data !

Dr. Horst PUSCHMANN

OlexSys/ U. Durham

From 8.30: Computer Set-up *We will assist with any installation problems*

9.00 - 10.30: Introduction to Olex2 *What is Olex 2 ? Getting started*

We will explore the Olex2 GUI (graphical user interface) and provide an overview of the capabilities of the software. The basic concepts behind Olex2 will be explained.

10.30-10.50: Coffee Break

10.50 - 12.20: A Structure Determination *A simple small molecule from start to finish*

We will perform a complete structure analysis of a small-molecule structure from solution, model-building and refinement (using olex2.refine and ShelXL-2013) through to the generation of an IUCr journal-ready CIF. The basics of the Olex2 workflow will be demonstrated.

12.20-13.40 Working Lunch: *Try what you've seen!*

A leisurely Chinese buffet lunch with Dim Sum provided, but there's time to try out some things you have seen…

13.40 - 15.10: Olex 2 Advanced Tools *Exploring more complicated cases*

- electron density maps
- split and fit fragments
- solvent masking
- advanced tools for model building
- import/export fragments
- disorder across symmetry elements

15.10-15.30 Afternoon Tea

15.30 - 17.00: Finishing with Olex2 *Tools for displaying and reporting structures*

The aim here is to give you an opportunity to experience what Olex2 is capable of and demonstrate some of the tools to grow and pack structures as well as producing images, reports and CIFs for publication.

OlexSys This workshop is run by OlexSys Ltd, Department of Chemistry, Durham University, UK.

We hope that you will be able to drive Olex2 well enough by the end of the day so that you can start looking at some of your own structures. So please bring some of your own data along to try !

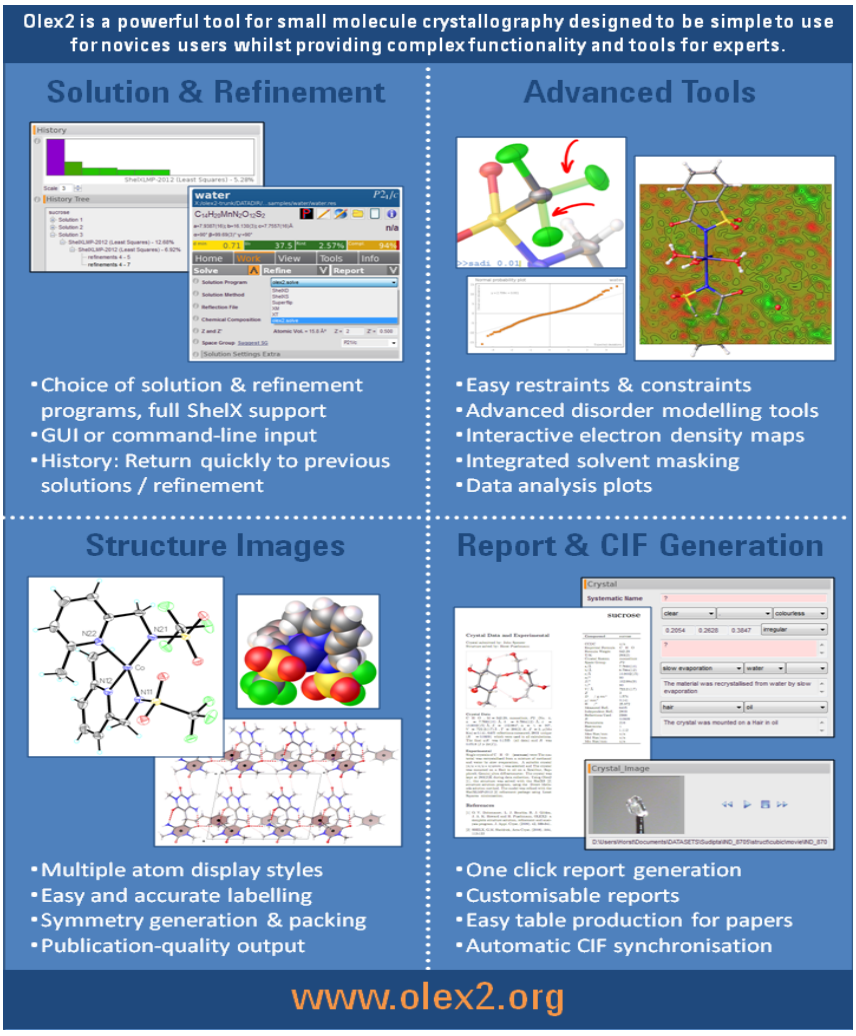
The Olex2 team led by Dr. Horst Puschmann will be at AsCA'13 throughout the conference – if you have any queries, problems, suggestions or just want to have a chat, please come and find us !

Olex2 Asian Workshop Registration

Please download the **Registration Form** indicate Olex2 as the preferred workshop and E-mail to asca13@ust.hk. (Gilbert: **Registration Form** add link to file Olex2_form.docx)

Background for Olex2

Before attending the conference you may visit the website www.olex2.org (hyperlink) for further details of the program and a free download http://www.olex2.org/download/ (hyperlink)



OlexSys This workshop is run by OlexSys Ltd, Department of Chemistry, Durham University, UK.