# Workshop #5: Simple and Advanced Single Crystal X-Ray Structure Refinement Using ShelXle

| | | | | |
|---|---|---|---|---|
| Date/Time | Friday, July 7, 2023 @ 10:00 AM ET | | | Registration Fees |
| Location | Essex C | | | Regular: $60 Per Person<br>Retired: $60 Per Person<br>PostDoc: $60 Per Person<br>Student: $60 Per Person |
| Max Capacity | 30 | | | |
| Main Contact | Matthias Zeller | | | |

## Description

ShelXle [1] is a graphical user interface for SHELXL [2], currently worldwide the most widely used program for small-molecule structure refinement, downloaded more than 70,000 times since its first release in 2011. ShelXle is fully compatible with all features of SHELXL and is written entirely in C++ using the Qt4/Qt5 libraries. It is available at no cost for Windows, Linux and Mac-OS X and as source code.



ShelXle combines an editor with syntax highlighting for the SHELXL-associated .ins (input) and .res (output) files with an interactive graphical display for visualization of a three-dimensional structure including high resolution the electron density (Fo) and difference density (Fo-Fc) maps. Editor (res file) and the graphical interface open at the same time, with instant simultaneous updating when making changes in either text or graphical editor. Special features of ShelXle include intuitive atom (re-)naming, support of PART and RESI commands as well as suffixes during atom renaming, unique and unrivaled structure visualization and highlighting tools, a symmetry manager supporting both EQIV and CIF style codes, as well as novel and unique ways of displaying disorder around both general and special positions. The DSR [3, 4] plugin can be of great help for modeling of complicated disorder. An intuitive hydrogen placement tool, atom sorting features, automatic unit cell content updating and removal of unused structure factors, and iterative weighting scheme optimization, tools for neutron and synchrotron data refinement and the ability to directly add or link additional external programs round out the capabilities of ShelXle.

In the workshop, attendees will go through worked examples that focus on both simple as well as advanced single crystal structure refinement using ShelXle. Topics will include the use of symmetry tools and difference density maps, structure visualization tools and disorder refinement, both with and without use of the DSR plugin. Attendees will be introduced to an easy-to-use interface to SHELXL and have a chance to discuss specific SHELXL or ShelXLe related questions and/or problems.

[1] C. B. Hübschle, G. M. Sheldrick and B. Dittrich, (2011) J. Appl. Cryst. 44, 1281-1284.
[2] G. M. Sheldrick, (2008). Acta Cryst. A64, 112-122.
[3] D. Kratzert, I. Krossing, (2018) J. Appl. Cryst. 51, 928-934.
[4] D. Kratzert, J. J. Holstein, I. Krossing, (2015) J. Appl. Cryst. 48, 933-938.

## Schedule*

| Time | Instructor/Topic |
|---|---|
| 10:00 AM - 10:15 AM ET | Installation: ShelXle |
| 10:15 AM - 11:00 AM ET | • Review of SHELXL<br>• Introduction to ShelXle: features and program structure<br>• Examples |
| 11:00 AM - 12:15 PM ET | Simple Structures Session |
| 12:15 PM - 12:30 PM ET | Wrap Up |
| 12:30 PM - 2:00 PM ET | Lunch (included) |
| 2:00 PM - 2:30 PM ET | Introduction to advanced features and challenging structures (disorder, twins, partial occupancy) |
| 2:30 PM - 3:30 PM | Challenging Structures Session |
| 3:30 PM - 4:00 PM | Discussion & Closing |

**Tentative and subject to change.*

**Quick Links**

ACA Homepage
Conference Attendee Guide
Oxford Abstracts Platform
Oxford Abstracts Poster Gallery
Full Program 2023
Oxford Abstract Platform Information

**Announcements**

Welcome to our newest ACA Fellows!

Three Minute Thesis Sponsors

Anton Paar

Opening Reception Sponsor

BIORTUS

Special Sponsors

Rigaku

ALTOS

YSIG Lunch Sponsor

AIP

Diamond Level Sponsors
[$5,000+]

Rigaku

BIORTUS

ThermoFisher SCIENTIFIC

Ruby Level Sponsors
[$2,500-$4,999]

Anton Paar

nanosoft

NEW ENGLAND BioLabs Inc. — be INSPIRED drive DISCOVERY stay GENUINE

Genentech
A Member of the Roche Group

MiTeGen
www.mitegen.com

AIP

MERCK
INVENTING FOR LIFE

SHUIMU

NSF's ChemMatCARS UCHICAGO

BRUKER

Emerald Level Sponsors
[$1,000-$2,499]

STRUCTURA BIOTECHNOLOGY

Poly Crystallography, Inc.

Structural Dynamics

DECTRIS
detecting the future

TESCAN

WYATT TECHNOLOGY

Nanome

SEISMIC THERAPEUTIC

xenocs
Exploring the very small

ALTOS

REFEYN

Sapphire Level Sponsors
[$1-$999]

GATAN
AMETEK

HELIX BIOSTRUCTURES

NIS
NANOIMAGING SERVICES

sptlabtech & quantifoil

WYATT TECHNOLOGY

diamond