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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 Retired: \$60 Per Person PostDoc: \$60 Per Person 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 Introduction to ShelXle: features and program structure 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.

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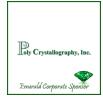
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