ShelXle

– a GUI for structure determination with SHELXL

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Content

- Introduction
- Main program functions
- Editor
- Running SHELXL (and SHELXT) within ShelXle
- Concluding remarks
  - Download, tutorial, citation

Introduction
- Comparison

XP

- Old
- Interacts with the user by 4 letter keywords

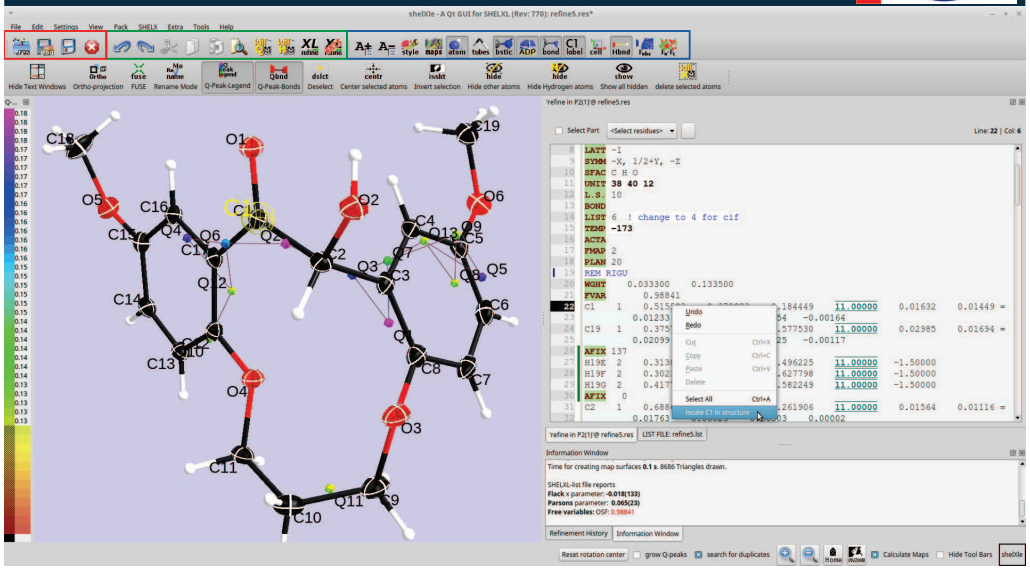
ShelXle

- Nice and new
- Some very useful functions
- Focused on refinement
- Full file control of .ins + .res file

Olex2

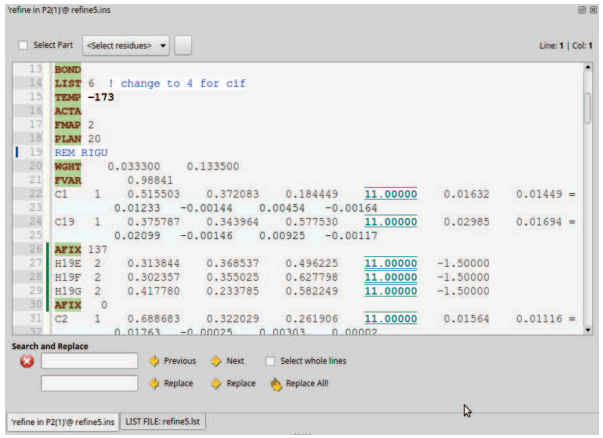
- Nice and new
- Many great functions and features
- All-in-one approach

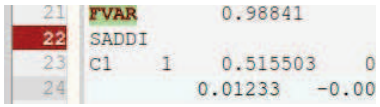
Main program functions

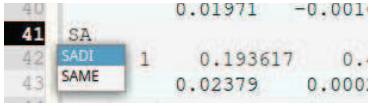


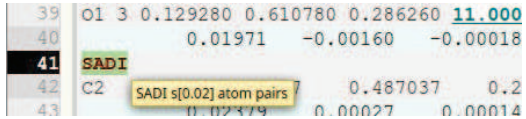
The Editor
Syntax highlighting & Search

- Comments
  - recognize !
  - REM (click)
  - block (right click)
- AFIX block
- Search (Ctrl + f)
- More common key combinations
  - (Ctrl +c, Ctrl + z, ...)









- Syntax errors:
  - lines not compatible with SHELXL
- Instruction completion
- Instruction syntax information with mouse

Running SHELXL in ShelXle

- Starting with solving the structure
  - Opening momo.ins mit Shelxle
  - Adding shelxt as external program
  - Running it and loading momo_a.res
- Running SHELXL (showing options), loading
- Renaming one molecule & running with ANIS
- Automatic HFIX 2x
- Refinement history
- Refine until WGHT converges, Screenshot resolution

Thanks

- Christian Hübschle
  - Writing this helpful program
  - Fixing bugs
  - Answering questions
- Daniel Kratzert
- Prof. G. Sheldrick

- Thank You for your attention.

Questions?

- Download:

  https://sourceforge.net/projects/shelxle/
  http://ewald.ac.chemie.uni-goettingen.de/shelx/

- Tutorial:

  http://shelx.uni-goettingen.de/MC3-tutorial/

- Publication to cite:

  Hübschle *et al., J. Appl. Cryst.,* ***44****, (2011) 1281-1284.*