



# ShelXle

## - a GUI for structure determination with SHELXL

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# 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

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# Main program functions



The screenshot displays the ShelXle GUI. The main window shows a 3D ball-and-stick model of a molecule with atoms labeled C1 through C19 and O1 through O6. The atoms are colored by element (Carbon in grey, Oxygen in red, Hydrogen in white). The interface includes a menu bar, a toolbar, and a command window on the right. The command window shows the following text:

```

value in F2117@ refine5.res
Select Part <Select residues>
Line 22 | Col 6
LAYER -1
SYMM -X, 1/2+Y, -Z
SFAC C H O
UNIT 38 40 12
L.S. 10
BOND
LIST 6 1 change to 4 for cif
TEND -173
ACTA
FMAP 2
SCALE 20
RSM RIGU
| WHIT 0.033300 0.133500
22 FVAR 0.38841
C1 1 0.3158 1.84449 11.00000 0.01632 0.01449 =
0.01233 B60 04 -0.00164 0.02985 0.01694 =
C19 1 0.3705 0.577530 11.00000
23 0.02099 25 -0.00117
AFIX 137
H19E 2 0.313 Stop CHC 4.96225 11.00000 -1.50000
H19F 2 0.302 Stop CHC 4.627798 11.00000 -1.50000
H19G 2 0.4177 Stop CHC 3.962245 11.00000 -1.50000
AFIX 0
C2 1 0.688 Rotate C1 H rotation 2.261906 11.00000 0.01564 0.01116 =
0.01763 03 0.00002
  
```

At the bottom of the screenshot, there is an information window with the following text:

```

value in F2117@ refine5.res | LIST FILE: refine5.lst
Information Window
Time for creating map surfaces: 6.1 x 8686 Triangles drawn.
ShelXle file reports
Flack + parameter: 0.018(133)
Parsons parameter: 0.065(23)
Free variables: 0/0 (0/0)
Refinement History | Information Window
Reset rotation center | grow Q peaks | search for duplicates |
  
```

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# 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, ...)

The screenshot shows the ShelXle editor window with a list of instructions on the left and a search and replace dialog box at the bottom. The instructions include BOND, LIST, TEMP, ACTA, FMAP, FIRM, REM, RIGU, WGHT, FVAR, C1, C19, AFIX, H19E, H19F, H19G, and C2. The search and replace dialog box has fields for search and replace text, and buttons for Previous, Next, Replace, and Replace All.

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```

22 C1 1 0.515503 0.372083 0.184449 11.00000 0.01632 0.01449 =
23 0.01233 -0.00144 0.00454 -0.00164
24 C19 1 0.375787 0.343964 0.577530 11.00000 0.02985 0.01694 0.02095
25 AFIX 137
26 H19E 2 0.313844 0.368537 0.496225 11.00000 -1.50000
    
```

```

21 FVAR 0.98841
22 SADDI
23 C1 1 0.515503 0
24 0.01233 -0.00
    
```

- Syntax errors:  
lines not compatible with SHELXL

```

40 0.01971 -0.001
41 SA
42 SADI 1 0.193617 0.
43 SAME 0.02379 0.000
    
```

- Instruction completion
- Instruction syntax information with mouse

```

39 O1 3 0.129280 0.610780 0.286260 11.000
40 0.01971 -0.00160 -0.00018
41 SADI
42 C2 SADI s[0.02] atom pairs 0.487037 0.2
43 0.02379 0.00027 0.00014
    
```

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# 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

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# Thanks



- Christian Hübschle
  - Writing this helpful program
  - Fixing bugs
  - Answering questions
- Daniel Kratzert
- Prof. G. Sheldrick
- Thank You for your attention.

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# 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.