



# ShelXle

– a GUI for structure  
determination with SHELXL

By Christian Hübschle

Claudia M. Wandtke, ACA Denver, 2016

# 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



shelXle - A Qt GUI for SHELXL (Rev: 770): refine5.res\*

File Edit Settings View Pack SHELXL Extra Tools Help

Q-Peak Legend Q-Peak-Bonds Deselect Center selected atoms Invert selection Hide other atoms Hide Hydrogen atoms Show all hidden delete selected atoms

refine in P2(1)@ refine5.res

Select Part <Select residues>

Line: 22 | Col: 6

8	LATT	-1							
9	SYMM	-X, 1/2+Y, -Z							
10	SFAC	C H O							
11	UNIT	38 40 12							
12	L.S.	10							
13	BOND								
14	LIST	6 ! change to 4 for cif							
15	TEMP	-173							
16	ACTA								
17	FMAP	2							
18	PLAN	20							
19	REM	RIGU							
20	WGHT	0.033300	0.133500						
21	FVAR	0.98841							
22	C1	1	0.515500	0.184449	<u>11.00000</u>	0.01632	0.01449	=	
23			0.01233	54	-0.00164				
24	C19	1	0.375	577530	<u>11.00000</u>	0.02985	0.01694	=	
25			0.02099	25	-0.00117				
26	AFIX	137							
27	H19E	2	0.313	496225	<u>11.00000</u>	-1.50000			
28	H19F	2	0.302	627798	<u>11.00000</u>	-1.50000			
29	H19G	2	0.417	582249	<u>11.00000</u>	-1.50000			
30	AFIX	0							
31	C2	1	0.688	261906	<u>11.00000</u>	0.01564	0.01116	=	
32			0.01763	303	0.00002				

undo redo cut copy paste delete select all

locate C1 in structure

refine in P2(1)@ refine5.res LIST FILE: refine5.lst

Information Window

Time for creating map surfaces 0.1 s. 8686 Triangles drawn.

SHELXL-list file reports

Flack x parameter: -0.018(133)

Parsons parameter: 0.065(23)

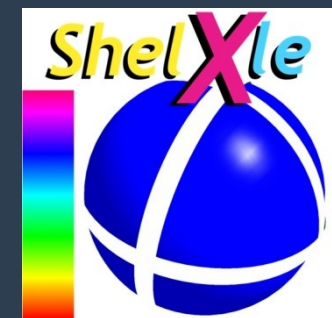
Free variables: OSF: 0.98841

Refinement History Information Window

Reset rotation center grow Q-peaks search for duplicates Calculate Maps Hide Tool Bars shelXle

# 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, ...)

```
'refine in P2(1)@ refine5.ins
```

Select Part <Select residues> Line: 1 | Col: 1

```
13 BOND
14 LIST 6 ! change to 4 for cif
15 TEMP -173
16 ACTA
17 FMAP 2
18 PLAN 20
19 REM RIGU
20 WGHT 0.033300 0.133500
21 FVAR 0.98841
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 =
25 0.02099 -0.00146 0.00925 -0.00117
26 AFIX 137
27 H19E 2 0.313844 0.368537 0.496225 11.00000 -1.50000
28 H19F 2 0.302357 0.355025 0.627798 11.00000 -1.50000
29 H19G 2 0.417780 0.233785 0.582249 11.00000 -1.50000
30 AFIX 0
31 C2 1 0.688683 0.322029 0.261906 11.00000 0.01564 0.01116 =
32 0.01763 -0.00025 0.00303 0.00002
```

Search and Replace

Previous Next  Select whole lines

Replace Replace Replace All

'refine in P2(1)@ refine5.ins LIST FILE: refine5.lst



```

22 C1 1 0.515503 0.372083 0.184449 11.0000 0.01632 0.01449 =
23 0.01233 -0.00144 0.00454 -0.00164
24 C19 1 0.375787 0.343964 0.577530 11.0000 0.02985 0.01694 0.0209
25 AFIX 137
26 H19E 2 0.313844 0.368537 0.496225 11.0000 -1.50000

```

- Syntax errors:

lines not compatible with SHELXL

- Instruction completion
- Instruction syntax information with mouse

```

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

```

```

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

```

```

39 O1 3 0.129280 0.610780 0.286260 11.000
40 0.01971 -0.00160 -0.00018
41 SADI
42 C2 0.487037 0.2
43 0.02379 0.00027 0.00014

```

# 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.