



## Practicals



In **ChemicalCrystallography.zip** you find

- a demo version of XPREP
- \*.p4p (cell dimension and formula)
- and \*.hkl of seven example structures

You should have installed

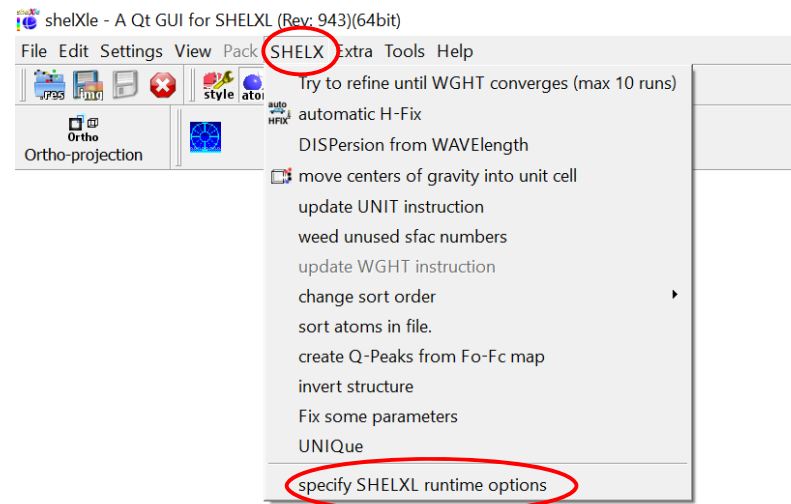
- all SHELX programs (SHELXS, SHELXD, SHELXL, SHELXT)
- PLATON
- Shelxle

Define in Shelxle the path for

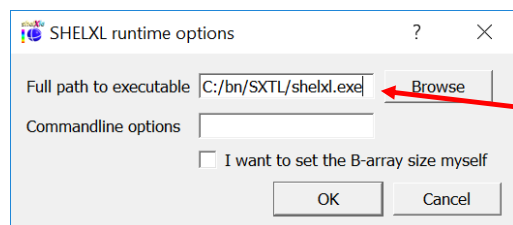
- SHELXL
- Platon



## Shelxle: Define SHELXL



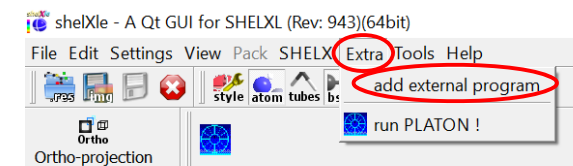
## Shelxle: Define SHELXL



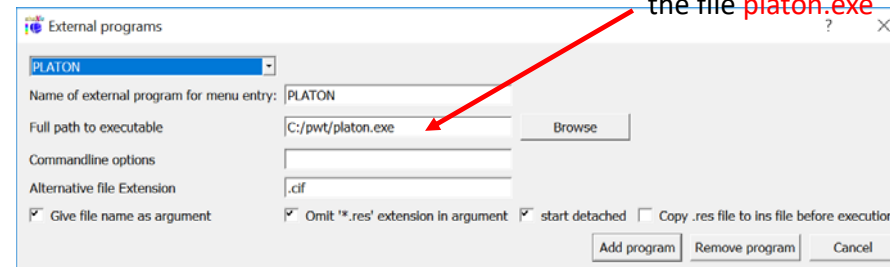
your directory with  
the file **shelxl.exe**



## Shelxle: Define Platon



your directory with  
the file **platon.exe**



## Practical Training on Twinning in Chemical Crystallography

### (Pseudo)(Reticular)-merohedral Twins

For every structure you have the following files:

1. \*.p4p cell constants and molecular formulae
2. \*.hkl reflection file

1. ANILIN: C<sub>6</sub> H<sub>7</sub> N  
21.645 5.833 8.319 90.00 101.12 90.00  
P. Müller, R. Herbst-Irmer, A. L. Spek, T. R. Schneider, M. R. Sawaya, Crystal Structure Refinement – A Crystallographer's Guide to SHELXL, Oxford University Press, 2006.
2. CITRO: C<sub>24</sub> H<sub>54</sub> O<sub>3</sub> Si<sub>3</sub>  
10.047 48.415 90.27 89.83 119.79  
R. Herbst-Irmer, G. M. Sheldrick, Refinement of obverse/reverse twins, Acta Crystallogr. B58, 477 (2002).  
P. Müller, R. Herbst-Irmer, A. L. Spek, T. R. Schneider, M. R. Sawaya, Crystal Structure Refinement – A Crystallographer's Guide to SHELXL, Oxford University Press, 2006.
3. HP33B: K Au (CN)<sub>2</sub>  
7.2397 7.2397 26.4450 90.0000 90.0000 120.0000  
R. Herbst-Irmer, Twinning in Chemical Crystallography – A Practical Guide, Z. Kristallogr., 231, 573 (2016).
4. CS: C<sub>15</sub> H<sub>20</sub> N Cs  
11.370 11.370 20.496 90.00 90.00 120.00  
R. Herbst-Irmer, Twinning in Chemical Crystallography – A Practical Guide, Z. Kristallogr., 231, 573 (2016).
5. ALUMONE: C<sub>27</sub> H<sub>26</sub> Al N<sub>2</sub> I  
16.9337 16.9337 12.6033 90.0000 90.0000 120.0000  
R. Herbst-Irmer, Twinning in Chemical Crystallography – A Practical Guide, Z. Kristallogr., 231, 573 (2016).
6. UWE48: C<sub>36</sub> H<sub>88</sub> Li<sub>4</sub> N<sub>4</sub> Si<sub>4</sub>,  
11.793 11.793 34.780 90.00 90.00 90.00  
L. Ruwisch, U. Klingebiel, S. Rudolph, R. Herbst-Irmer, M. Noltemeyer, (Di-tert-butylmethylsilyl)-amide - a Building Block for Azasilacyclobutane Synthesis, Chem. Ber. 129, 823 (1996).
7. MELLING: C<sub>72</sub> H<sub>60</sub> P<sub>3</sub> Os O  
12.623 12.623 26.325 90.00 90.00 120.00  
R. Herbst-Irmer, G. M. Sheldrick, Refinement of Twinned Structures with SHELXL97, Acta Crystallogr. B54, 443 (1998)  
P. Müller, R. Herbst-Irmer, A. L. Spek, T. R. Schneider, M. R. Sawaya, Crystal Structure Refinement – A Crystallographer's Guide to SHELXL, Oxford University Press, 2006.