

HOW TO'S FOR SOLVING PROBLEMS/TASKS WITH PLATON

1 – How to SQUEEZE with SHELXL2014

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3 – How to RENAME atom labels in a .res file

1 – How to SQUEEZE with SHELXL2014

1. Refine a non-disordered solvent model (i.e. excluding the solvent that needs to be 'modelled' by SQUEEZE) with the files **<name>.ins** & **<name>.hkl** to convergence (Include the ACTA instruction). The result will be the files **<name>.cif** and **<name>.fcf**. Do not remove the embedded **.res** and **.hkl** files!)
2. Run PLATON/SQUEEZE in a terminal window based on the **<name>.cif** & **<name>.fcf** files produced in step 1 with the command '**platon -q <name>.cif**'. The result will be the files **<name>_sq.ins**, **<name>_sq.hkl** & **<name>_sq.fab**. The **<name>_sq.fab** file includes the solvent contribution to the calculated structure factors (details of the SQUEEZE calculation are embedded in this file as well). Inspect the listing file **<name>_sq.lis**.
3. Continue SHELXL refinement in the presence of the files **<name>_sq.ins**, **<name>_sq.hkl** & **<name>_sq.fab** from step 2 with the command '**shelxl <name>_sq**'
4. Inspect the list files and validate (i.e. run '**platon -u <name>_sq.cif**'). The result will be in the files **<name>_sq.chk** & **<name>_sq.ckf**).

Notes:

a) Changes to the above in case of disordered solvents + Twinning:

The FCF produced in step 1 should be in that case of the 'LIST 8' type. This is needed to allow PLATON/SQUEEZE to run based on twin deconvoluted reflection data (Note: the SHELXL refinement in step 3 will again be based on the twinned data). The **<name>.ins** file should include the ACTA, LIST 8, BASF and TWIN or HKLF 5 instructions

b) Generally, no recycling of steps 1 to 3 will be needed. However, to accomplish this, it is possible to start with the **<name>.cif** & **<name>.fcf** from step 1 and run PLATON/SQUEEZE with the command '**platon -qn <name>.cif**' where 'n' is the number of cycles.

c) There should be no residual unresolved (disorder) density in the discrete model part of the structure because of its impact on the quality of the difference map in the solvent region. The dataset should be reasonably complete and with sufficient resolution [i.e. $\sin(\theta)/\lambda > 0.6$]. There should be no unresolved charge balance issues that might effect the chemistry involved (e.g. the valency of a metal in the ordered part of the structure). The reported electron count in the solvent region is meaningful only with the supply of a complete and reliable reflection data set. The SQUEEZE technique can not handle properly cases of coupled disorder effecting both the model and the solvent part of the structure. The solvent region is assumed not to contain significant anomalous scatterers.

2 – How to apply a unit cell transformation to a SHELXL .ins file

What is needed is the insertion into the <name>.ins of a record with the general format:

TRMX m11 m12 m13 m21 m22 m23 m31 m32 m33 t1 t2 t3

where **m11,m12,...,m33** are the 9 components of the cell transformation matrix and **t1,t2,t3** the components of the optional origin shift after transformation.

Such a record will generally be inserted directly after the TITL record. The effect will be that the transformation will be applied on what follows, i.e. the cell parameters, the space group, the coordinates and the displacement parameters. A proper transformation matrix will be inserted on the HKLF record. In such a way, no explicit transformation of the reflection file (<name>.hkl) will be needed for the subsequent SHELXL refinement.

Implementation:

Start terminal window

Edit <name>.ins to include the TRMX record

Invoke: 'platon <name>.ins (where <name> is substituted by the actual filename)

Click on 'Create-res (on the Main Menu under MISC-TOOLS)

As a result, a new <name>.res file is created

Notes:

- The TRMX command may also represent a unit cell halving etc.

3 – How to RENAME atom labels with PLATON in a .res file

1. start PLATON with the command '**platon -r <name>.res**'.

2a. Hit return (the graphics window should be active). The program will loop over all atoms in sequence with the current label changed from white to red. Hitting return will leave the label as indicated and the new in line label will turn red. Otherwise a new label name can be entered.

2b. Click on the atom for the label has to be changed and enter the new name.

Notes:

a) Atom labels that have been changed turn green

b) In case of a conflict with a label name that is already present, the already present atom label will be changed in a new label (that can be changed later on)

c) when finished, click on 'END'. The new RES file will be on **<name>_new.res**