HOW TO'S FOR SOLVING PROBLEMS AND TASKS WITH PLATON

INDEX (Version 22 Oct 2018)

1 – How to Update to the Latest PLATON Version

PLATON is regularly updated. The version date of the installed version is displayed on the main PLATON menu. When a new version of the source code is available on the WEB, that will be displayed in RED next to the installed version data. For this to work, the computer has to be on the Internet with the 'curl' utility installed. Alternatively the following WWW WEB-address can be consulted: http://www.platonsoft.nl/xraysoft/update_history_platon.html . New source code versions for UNIX (LINUX, MAX-OSX) can be downloaded from http://www.platonsoft.nl/xraysoft. The latest MS-windows executables are available from http://www.chem.gla.ac.uk/~louis/software/platon.

For UNIX (LINUX, MAC-OSX), the source code of the latest PLATON version can be downloaded conveniently (in the current directory) by clicking in the RED new-version area. GFORTRAN and GCC (or similar) will be needed to compile platon.f and xdrvr.c respectively. The compile command should look something like:
'(sudo) gfortran -o platon platon.f xdrvr.c -L/usr/X11R6/lib -lX11'.

See http://www.platonsoft.nl/xraysoft/Mac-OSX/platon/Platon_installation_on_a_Mac.pdf for detailed installation instructions on a Mac.

2 – How to run PLATON/SQUEEZE together with SHELXL2014

The PLATON/SQUEEZE tool can be used to calculate the scattering contribution to the calculated structure factors of disordered solvent(s) in a crystal structure as part of the the least-squares refinement of an otherwise parametrized structure.

Reference: Spek, A.L. (2015). Acta Cryst. C71, 9-19.

The SQUEEZE procedure is as follows (assuming that the non-solvent part of structure is complete, including hydrogen atoms)

Step 1:. Refine the disordered solvent free model (i.e. exclude any solvent that needs to be 'modelled' by **PLATON/SQUEEZE**) using **SHELXL2014** with the files **<name>.ins** & **<name>.hkl** to convergence (Include the **ACTA** instruction to create a LIST 4 type FCF file). The result of the calculation will be the files **<name>.cif** and **<name>.fcf**. Do not remove the embedded **.res** and **.hkl** files from the resulting CIF !). The averaged observed reflections in the FCF are used only in step 2.

Step 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). The **<name>_sq.ins** & **<name>_sq.hkl files** are copies of the embedded .res & .hkl from the step 1 calculation. The ABIN instruction is added to the INS file and the L.S. command is modified. Inspect the listing file **<name>_sq.lis**.

Step 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**'

Step 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.

3 – How to Validate a Crystal Structure

X-Ray crystallography has rightly the name of providing SOLID information on molecules in the crystalline state. However, the often forgotten condition to justify such a label for a particular instance of a crystal structure determination is that the underlying procedures should have been carried out adequately and correctly. Unfortunately, that is not always the case. Major causes are related to lack of experience in picking up signals indicating problems. Objective validation procedures attempt to address a large number of potential problems as a routine procedure (A.L.Spek,J.Appl. Cryst, 36, (2003), 7-13 and A.L.Spek, Acta Cryst. D65, (2009), 148-155).

The proper starting point for a meaningful structure validation are the CIF and FCF files. The FCF file contains the merged reflection data on which the interpretation as presented in the CIF is based. Many questions that arise as part of the structure validation can only be addressed with availability of the reflection data. The latest SHELXL refinement program archives automatically the unmerged reflection data in the CIF. In that case no additional FCF data need to be supplied.

PLATON contains the CheckCIF facility that is also used by the IUCr CheckCIF server. The validation test criteria with associated information is stored in an external file (**check.def**). A proper copy will be installed in the current directory where PLATON is run when such a file is not found or accessible. Structure validation of the data in **<name>.cif** can be invoked with the terminal command '**platon -u name.cif'.** The result of the analysis will be in two files: **<name>.chk** and **<name>.ckf**. The first file is the main report. The second file analyses in particular the reflection data.

Validation can also be invoked from the PLATON main menu by clicking on '**Validation**' or '**FCF-Valid**'.

4 – How to apply a unit cell transformation to a SHELXL INS/RES 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>_pl.res** file is created

Notes:
- The TRMX command may also represent a unit cell halving etc.
- Certain instructions such as those for constraints & restraints are not copied. They will have to be added again.

5 – How to move molecules with there center-of-gravity within the bounds of the unit cell

It is good practice to report structures with all molecules with their center-of-gravity within the bounds of the crystallographic unit cell. Exceptions may be molecules such as water that are best positioned on hydrogen bonding distance from the main molecule.
This operation is easily performed with the PLATON/Create-RES menu option in the early stage of the structure refinement, based on a .ins or .res file. The result will be a ._pl.res file.
By default, the molecule out of the set of symmetry related one's will be chosen that is closest to the origin at (0,0,0). That choice can be changed to e.g. (0.5,0.5,0.5) with the keyboard instruction **'NOMOVE OFF 0.5 0.5 0.5'** prior to the 'Create-RES' menu instruction.

6 – How to RENAME atom labels with PLATON in an INS/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>_pl.res**

7– How to order and Auto-Rename atoms in a CIF or INS/RES file

The keyboard instruction **platon -R <name>.cif** or **platon -R <name>.res** will produce the file **<name>_pl.res** with the atoms sorted per residues and with the atoms relabeled in a reasonable order
The same can be achieved by clicking on the Auto-Rename option on the PLATON main menu. The thus created RES file might need some further editing.

8 – How to calculate the Kitaigorodskii Packing Index

A crystal structure without room for embedded solvents of crystallization will still include small volumes outside of the van der Waals radii of the atoms making up the structure. A measure for the volume taken by the atoms is the (Kitaigorodskii) Packing Index. This value will generally be in the order of 65%..

The value of the Packing Index for a given structure (as an INS or CIF file) can be calculated by clicking on the PLATON main menu function '**CALC K.P.I**'. This calculation is part of a search for solvent accessible voids (which should be very small or absent for a meaningful P.I.)

9 – How to apply a unit cell transformation to a SHELXL.hkl file

In general, there is no need to transform the reflection file data after a unit cell transformation. That transformation will be applied automatically by SHELXL when the relevant transformation matrix is supplied in the HKLF record. In that way there is only one copy of the reflection file.

The following options in PLATON are available in PLATON to carry out a 'hard' transformation of the reflection file:

1 – Startup PLATON with the relevant **<name>.ins** & **<name>.hkl** as '**platon name.ins**' and click on the PLATON main menu option '**HKL-Transf'.** The result will be the file **<name>_trans.hkl.** Also, a new **<name>_trans.ins** will be created with the (implicit) unit matrix in the the HKLF record.

2 – Placing a 'HKLT' record after the HKLF record in the .ins has the same effect as with option 1.

10 – How to generate an ab-initio HKLF4 reflection file for test purposes from a RES or CIF file

Sometimes, an ab-initio HKLF4 style reflection file with 'observed' data generated from the coordinates and displacement parameters present in a supplied **.ins**, **.res** or .**cif** can be useful for program(ming) test purposes. This can be accomplished with the **HKLF-Gener** tool on the PLATON main menu. The generated dataset will comprise the asymmetric part of the reflection

sphere with systematic absences removed. Artificial sigma(I)'s are calculated as **Sig(I) = MAX(0.01, SQRT(I) + 0.02 * I)**.
Data are generated within the 'Copper Sphere' (i.e. sin(theta)/lambda = 1/1.5418 = 0.65 Ang-1). To set the resolution to 0.6 Ang-1: **SET PAR 540 0.6.** Reflection data (SHELXL HKLF 4 format) are written to a file with extension **_gener.hkl**. I and sig(I) are written as integers but are on absolute scale when read as (3I4,2F8.2).

Note: The alternative keyboard instruction is (The menu default is **ASYM GENERATE**):

ASYM (AVF) GENERATE

The **AVF** keyword determines whether or not for non-centrosymmetric space groups the Friedel related reflections will be averaged (i.e. for the monoclinic space group P21 half a sphere of data or one quarter will be generated).

11 – How to calculate Least-Squares planes and plane-plane, plane-line or line-line angles interactively

Various geometrical calculations can be performed interactively by invoking tools available from the PLATON main menu. Clicking on either **L.S.-plane**, **DihedAngle**, **AngLsplLin** or **AngleLines** will bring up an ORTEP view on which the relevant atoms can be clicked. The displayed molecule can be rotated to a suitable orientation when needed to get an optimal unobscured view.. Associated derived parameter su's are included when su's are supplied with the coordinate data (e.g. as a CIF). Atoms are treated with unit-weight in the least-squares plane calculation by default. Alternatives are weighting based on atomic weights and standard deviations (esd, su). The weighting scheme may be changed using the (UAE)WLSPL button. The result of the calculation is shown both on the graphics window, the terminal window and on the listing file.

*Interactive calculation of least squares planes with the **L.S.-Plane** tool.*

*T*he red menu item **LsplDistEnd** in the options menu (with three sub-boxes) on the right indicates that the program is ready to receive the names of the atoms that will determine the least-squares plane of interest by clicking on the corresponding atom centers. This sequence should be terminated (and the calculation initiated) by clicking in the **End** field in the red menu item. Atoms defining the least-squares plane may be separated from additional atom labels for which only the distance to the plane has to be calculated by clicking in the Dist field between the clicks on atoms. Alternatively, an instruction similar to **LSPL c3 c4 c5 DIST c1** could be issued from the keyboard.

Interactive calculation of dihedral angles between least squares planes with the DihedAngle tool.

The red menu item **LsplWithEnd** in the options menu on the right indicates that the program is ready to receive the atom names that will determine the first least-squares plane by clicking on the corresponding atom names. This sequence is ended and the sequence for the second plane started by clicking in the **With** side-menu box. The second sequence is ended (and the calculation initiated) by clicking in the **End** field. Alternatively, an instruction similar to **LSPL c3 c4 c5 WITH c1 c2 c6**

could be issued from the keyboard.

Interactive calculation of the angles between a least squares plane and a bond with the AngLsplLin Tool.

The red menu item **LsplWithEnd** in the options menu on the right indicates that the program is ready to receive the atom names that will determine the least-squares plane by clicking on the corresponding atom names. This sequence is ended and the sequence for the two bond atoms started by clicking in the **With** side-menu box. The second sequence is ended (and the calculation initiated) by clicking in the **End** field. Alternatively, an instruction similar to **LSPL c1 x2 c3 c4 with c5 c6** could be issued from the keyboard.

Interactive calculation of angle between two lines with the AngleLines tool.

The red menu item **Angle2Lines** in the options menu on the right indicates that the program is ready to receive the atom names that will determine the two lines respectively by clicking on the four atom names of the two lines/bonds.Alternatively, an instruction similar to **ANGLE c1 c2 c3 c4** could be issued from the keyboard.

12 – How to get the Hall symbol for a given symmetry and other symmetry related issues

PLATON includes a build-in space group symmetry handler with multiple functions. Several of those functions can also be used interactively without the need to supply coordinate or reflection data.

a) The terminal command **platon spgr 'P212121'** will report the Hall symbol and an explicit list of symmetry operations for space group P212121.

b) The terminal command **platon Hall '-P 2yab'** will report the H-M symbol (when in a known setting) and an explicit set of symmetry operations.

c) The terminal instruction **platon spgr** gives access to the other options: e.g. the option to build up the set of symmetry operators with **LATT** and **SYMM** input records followed by a **LIST** instruction. Note: only the subset of space group generators will be needed.

13 – How to recover an INS and HKL file from a shelxl.cif (+ shelxl.fcf)

A **.ins** and **.hkl** might be needed for additional calculations on a published structure. With SHELXL2014 and up those files are embedded in the CIF and can be extracted with the **shredcif** utility that is provided with the SHELX distribution. Alternatively, recovering those files can be accomplished with the terminal window instruction **platon -H <name>.cif**. The result will be two

files: **<name>_sx.ins** and **<name>_sx.hkl** (and where applicable, <**name>_sx.fab** and **<name>_sx.fcf**). In most other cases (e.g. with a **shelxl97** based CIF) also a **<name>.fcf** will be needed. A **<name>_sx .ins** file will in that case be created from the data in the CIF and a **<name>_sx.hkl** file from the observed data in the **<name>.fcf**. The latter file includes necessarily only the merged reflection set and does not include the systematically absent intensities.
The **cif2shelxl** tool on the PLATON main menu has the same effect as the -H switch on the command line. The **cif2shelxl** tool should be used for the extraction of individual entries from a multi-entry CIF.
Just click on ENTRY-LIST to get a display of all the entries in the CIF and click on the appropriate entry.

14 – How to discover and visualize solvent accessible voids

Solvent accessible voids in a structure (available as cif, res, ins, spf) can be reported with the **calc solv** and **calc void** tools from the PLATON main menu. The calc solv version is faster and does not report the Kitaigorodskii packing index.
Visualisation of the voids in the unitcell is possible either with the **Solv Plot** or **CavityPlot** tools from the PLATON main menu. The former plots the surface of the solvent accessible void. The latter fits spheres withing the voids.

15 – How to get Anomalous Dispersion Parameter Values

Anomalous dispersion parameter values (f', f" and contribution to mu) are tabulated in the International Tables for common K-alpha wavelength's. For other wavelength's (generally from a synchrotron radiation source) a build-in PLATON tool can be used:
Start PLATON as '**platon -**' (thus including the space + dash characters) and issue the command **ANOM <wavelength>** (e.g. **ANOM 0.8**). The result will be a graphical output and a listing of the dispersion parameters for all elements on the terminal window. Other instruction options are **ANOM <element>** and **ANOM <element> <wavelength>**.

Alternatively, for just a listing of f', f'' and mu values for elements 1 to 92 for a given wavelength, issue the terminal command **platon ANOM <wavelength value>**. The result is available in the file ANOM_Brennan_Cowan.lis and in the terminal window.

The dispersion parameter values are calculated following S.Brennan & P.L.Cowan (1992).Rev.Sci.Instr., 63, 650.