Installing and running X-ray solution and refinement software on a MacOS computer

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Summary

Not all software packages commonly used for solving and refinement of small molecule single crystal X-ray structure analysis are available for Linux, Windows and Mac OS. This guide will walk you through setting up a MacOS computer to solve and refine X-ray crystal structures using the some of the most common program packages. Installation of many of these software packages on a MacOS computer is not very user friendly. This document is ordered from easy software to difficult software to install. The first packages are easy to install, and use graphical installers. The later packages require the use of the command line. You will need to know how to do basic file manipulation (`ls`, `cd`, `mv`, `cp`) on the command line for the later packages. Towards the end of the document you will find some guidelines how to use the software once installed.

The packages that you will be installing are: XQuartz, ShelXLE, Mercury, Conquest, Homebrew, Wine, ShelX, xprep, and Platon. ShelXLE, Mercury, Conquest, ShelX, xprep, and Platon are dedicated X-ray analysis packages. XQuartz, Homebrew and Wine are needed to get all of the packages running on your MacOS computer.

Easy Stuff: XQuartz, ShelXLE, Mercury, Conquest

First, the easy stuff:

1. You will need the X11 server XQuartz to use most of this software. This is just a software package that displays windows on your screen for UNIX applications. Obtain it from https://www.xquartz.org . Be sure to log out and then back in to enable the X11 server.

2. There is a Mac version of ShelXLe available. This is the graphical user interface (GUI) that you will use to solve crystal structures (it runs the ShelXL refinement executable in the background). Obtain ShelXLe from: https://www.shelxle.org/

3. There is a Mac version of the Cambridge Structural Database, which comes with both Mercury and Conquest. These are software packages that you will use to visualize crystal structures and to search for already published structures. Uninstall Mercury if you have a standalone version already installed, and then obtain the package from Matt. (You can skip this one if you don't have room for it on your hard disk; a full CSD installation requires > 6 GB disk space; there is an online version of the CSD which is almost as good. In that case, you can use the Mercury standalone version, which is available for free online.)

Homebrew Installation

To install the remainder of the software, you'll need to install some dependencies first. These can be obtained by using Homebrew. To install homebrew, open Terminal.app and run the following command:

```
/usr/bin/ruby -e "$(curl -fsSL
https://raw.githubusercontent.com/Homebrew/install/master/install)"
```

This will download and install the homebrew software on your Mac. You can then use the homebrew package to install the software packages that you will need to run the X-ray software. You will need `wine`, which is a windows emulator, and `gcc`, which provides libgfortran. We'll also install `wget` because it's awesome. Run this command:

```
brew install wine gcc wget
```

ShelX Installation

The next software package you'll need is ShelX. This package includes, most importantly, the `shelxl` command, which is the program for crystal structure least squares refinement, as well as several other "Shelx" executables (ShelXS and ShelXM for structure solution, etc). Deal with the cumbersome registration process (there is no cost for academic users) and download all of the Mac bz2 files from: http://shelx.uni-goettingen.de/download.php. (The link to download the software is at the bottom of the page.)

Once you have the `.bz2` files, create a new directory in your home directory called "`bin`". Place all of the bz2 files that you downloaded in this "`bin`" directory. Open up Terminal.app and use these three commands to change into the bin directory, unzip all of the files, and make them executable:

```
cd bin
bunzip2 *.bz2
chmod 755 ./*
```

We can also add the bin directory to your default PATH, to make using these utilities easier:

```
echo "export PATH=\"\$PATH:~/bin/\"" >> ~/.bash_login
ln -s ~/.bash_login ~/.bashrc
source ~/.bash_login
```

Now, use the command "`cd`" to change back to your home directory, and try running the `shelxl` command. You should see some instructions about how to use the shelxl program. If it says that the command is not found, then there is a problem with your $PATH variable.

xprep Installation

Next, we'll install the Bruker utilities, including `xprep`. These programs are only available for Windows , so you'll need to install them with wine. Obtain the installer from the Purdue Crystallography lab, and then run it with wine:

```
wine ./BrukerAXSExecutables2009.9.exe
```

Sometimes this installer hangs, and so you may have to kill it with CTRL-C on the command line and then run it again. It should ask you for the serial number during the installation. The Purdue Crystallography lab has the serial number. Please note that this package is licensed to Purdue, so use is limited to Purdue users. Once the installation is completed, you should be able to run `xprep` with this command:

```
wine ~/.wine/drive_c/BN/SXTL/xprep.exe
```

You can create a shortcut to this command in your .bash_login file:

```
echo "alias xprep=\"wine ~/.wine/drive_c/BN/SXTL/xprep.exe\"" >> ~/.bash_login
source ~/.bash_login
```

Afterwards, you should be able to run `xprep` with just the `xprep` command:

```
xprep
```

Platon Installation

The last piece of software, Platon, is optional, but recommended. It's also probably the most difficult to install. At this point, you should have all of the software necessary to install it.

Platon is helpful with detecting and fixing twinning and missed or higher symmetry, or ill-defined solvate regions ("Squeeze"). You have to download and compile it:

```
wget http://www.cryst.chem.uu.nl/spek/xraysoft/unix/platon/platon.f.gz
wget http://www.cryst.chem.uu.nl/spek/xraysoft/unix/platon/xdrvr.c.gz
gunzip *.gz
gfortran –o platon platon.f xdrvr.c –I/opt/X11/include –L/opt/X11/lib –lX11
chmod +x ./platon
mv ./platon ~/bin/
```

You should be able to place the newly-compiled platon executable in your ~/bin directory, as shown, and then run it with the `platon` command.

Crystal Structure Solution Process

Now that you have all of the software installed, the basic structure solution process is similar to the process on windows:

1. After integration and scaling (done on the instrument computers), download the files name.abs, and name_0m._ls, .p4p, and .hkl from the work directory from the diffractometer hard drive (you can also copy the entire work folder). The easiest way to do this is by using your Purdue network drive, or by USB flash drive.
2. Use `cd` to change to the work directory, and run `xprep`. For example, if your hkl file is called MB8100A_0m.hkl, then type: `xprep MB8100A_0m` Follow the xprep instructions.

3. Use shelxs or shelxm on the command line to solve the structure: `shelxs MB8100A_0m` or `shelxm MB8100A_0m`

4. Use shelxle to open the resulting res file and solve the crystal structure.

Remote Access to the Diffractometers

Approved users can access the diffractometers remotely by using the built-in Screen Sharing utility. Just press command-space, launch Screen Sharing, and then type in the appropriate IP address and password. Please contact the Purdue Crystallography lab for access privileges and login credentials.