

Instructions for Setting Up Freeware Crystallographic Software

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SETTING UP CRYSTALLOGRAPHIC SOFTWARE ON WINDOWS

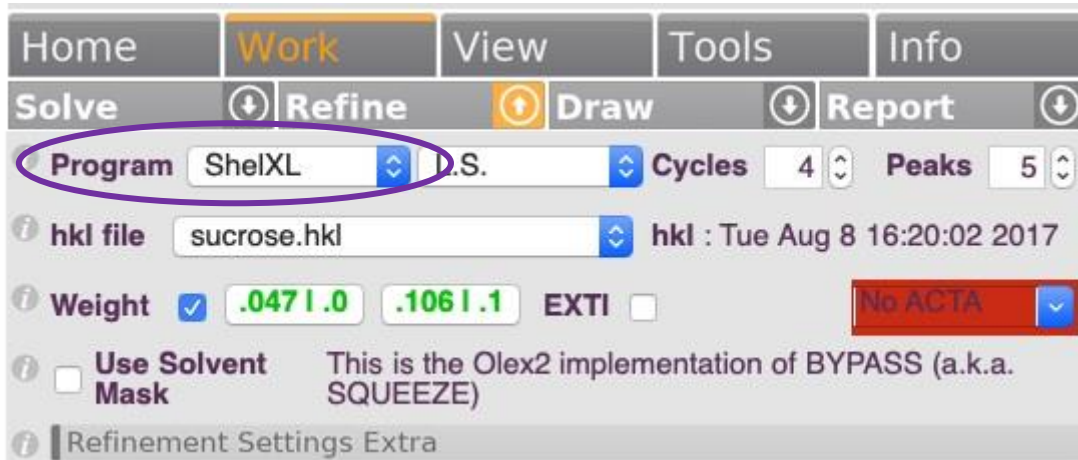
A. OLEX2

1. Download the Olex2 installer for Windows from either:
 - (if applicable) Canvas or OneDrive,
 - 'imsercdata' server under 'public/Crystallography/Olex2/Windows'. Read more information about connecting to the 'imsercdata' server under 'Data Access' at <http://imserc.northwestern.edu/about-general-faq.html#data>, or
 - The Olex2 website (<https://www.olexsys.org/olex2/>)
2. Install the downloaded file by double pressing on the EXE installer and following the installation GUI
3. If Olex2 prompts you to accept new updates, do this. Look at the bottom of the Olex2 window to check the update progress. Once it is finished updating, close Olex2 and re-open it for the changes to take effect

B. SHELX SOLUTION AND REFINEMENT PACKAGES

1. Download the SHELX for Windows file from either:
 - (if applicable) Canvas or OneDrive,
 - 'imsercdata' server under 'public/Crystallography/SHELX/Windows'. Read more information about connecting to the 'imsercdata' server under 'Data Access' at <http://imserc.northwestern.edu/about-general-faq.html#data>, or
 - Browse to the Shelx website (<https://shelx.uni-goettingen.de/>)
 - i. Fill out the registration information to get the download password
 - ii. Follow the links to download the files
2. Once downloaded, double press on the EXE file to install the software. Note the 'Destination folder' for the files in case you want to use SHELX through other software packages beyond Olex2
3. Make the ShelX files visible to Olex2. You have two options for this step depending on your choice of using SHELX through either Olex2 only ([section 3a](#)) or other software packages, e.g., ShelXle ([section 3b](#)):
 - a. [Olex2 only and faster to setup] Copy the EXE files from the 'Destination folder' (step #2) to the Olex2 installation folder and restart Olex2 if it is running. Olex2 should have the ShelX* options (see example in the figure below) available under the corresponding 'Program' drop-down menus under the 'Solve' and 'Refine' tabs (press on the icon with the circled arrow next to 'Solve' and 'Refine' to see all options)

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- b. [Other software packages] If the 'Destination folder' selected in step #2 is not part of the Path variable of Windows, you need to add the 'Destination folder' to the Path:
 - i. On the windows search, type 'variables' and select the 'Edit the system environment variables' option
 - ii. Press on the 'Environment Variables' button
 - iii. There are two variable sections, User variables and System variables. Select 'Path' under the system variables and press on the 'Edit' button
 - iv. Press on the 'New' button and the 'Browse' button and browse to the 'Destination folder' selected on step #2. Press 'OK'
4. Open up Olex2 and check to see if the ShelX programs are available under 'Solve' and 'Refine'. If the ShelX programs are not visible close Olex2 and reopen it. Run a refinement and a solution to be sure they work by pressing on the gray tab labeled as 'Refine' and 'Solve'. A successful refinement run should give you some numbers for R1 and wR2. A successful solution run should give you some atoms in the main view

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C. PLATON

1. Download Platon for Windows from either
 - a. (if applicable) Canvas or OneDrive,
 - b. 'imsercdata' server under 'public/Crystallography/Platon/Windows'. Read more information about connecting to the 'imsercdata' server under 'Data Access' at <http://imserc.northwestern.edu/about-general-faq.html#data>, or
 - c. From <http://www.platonsoft.nl/xraysoft/mswindows/platon/> download 'platon.zip' and 'pwt-setup.zip'
2. Make the Platon EXE file visible to Olex2. You have two options for this step depending on your choice of using Platon through either Olex2 only ([section 2a](#)) or other software packages, e.g., Platon Tool Bar ([section 2b](#)):
 - a. [Olex2 only and faster to setup] Unzip all files from 'platon.zip', and copy all files (EXE, DLLs, etc.) to the installation folder of Olex2. Platon can be run within Olex2 by pressing on the Platon icon at the top right corner of the Olex2 window (see circle in the figure below). Press on the Platon icon and the Platon window should pop up if installation was successful



The screenshot shows the Olex2 interface for a sucrose structure. The title bar reads 'Sucrose' and the path is '/Users/chris/Library/Application'. The chemical formula is $C_{12}H_{22}O_{11}$. The unit cell parameters are $a = 7.7727(9)$, $b = 8.7216(11)$, $c = 10.8637(11)$, $\alpha = 90^\circ$, $\beta = 102.983(11)^\circ$, $\gamma = 90^\circ$, $Z = 2$, $Z' = 1$, and $V = 717.63(15)$. The R-factors are $R_1 = 3.48\%$ and $wR_2 = 8.85\%$. The d min (Mo) is 0.73, $I/\sigma(I)$ is 32.7, R_{int} is 3.39%, and the full range is 50.5° to 99.7%. The shift is 0.002, Max Peak is 0.4, Min Peak is -0.3, and GooF is 1.046. The twin law is $(-1.0, 0.0, 0.0, 0.0, -1.0, 0.0, 0.0, 0.0, -1.0)$ with BASF [0.9(10)]. The structure is sucrose.

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- b. [Other software packages] Unzip 'pwt-setup.zip' and install the software by double pressing on the EXE installation file. Note the 'Destination folder' for this installation (default is 'c:\pwt'). If the installation folder selected is not part of the Path variable of Windows, you need to add the installation folder to the Path variable:
- i. On the windows search, type 'variables' and select the 'Edit the system environment variables' option
 - ii. Press on the 'Environment Variables' button
 - iii. There are two variable sections, User variables and System variables. Select 'Path' under the System variables and press on the 'Edit' button
 - iv. Press on the 'New' button and the 'Browse' button and browse to the installation folder selected on step #2. Press 'OK'
 - v. Unzip the 'platon.zip' and move the 'platon.exe' file into the installation folder selected on step #2. This step is required every time you want to upgrade Platon to the latest version
 - vi. Double press on the Platon EXE file to ensure that Platon starts properly, and no errors appear
 - vii. If using Platon through Olex2, restart Olex2 if running and check to see if the Platon icon appeared at the top right corner of Olex2 (see circle in the figure above)

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SETTING UP CRYSTALLOGRAPHIC SOFTWARE ON MACOS

This guide was updated for Big Sur, Catalina, and should work on High Sierra as well. This guide might require temporarily disabling the security integrity protocol and editing the '/usr/bin' folder. With any software installation, it is advisable to back up your files before proceeding.

A. OLEX2

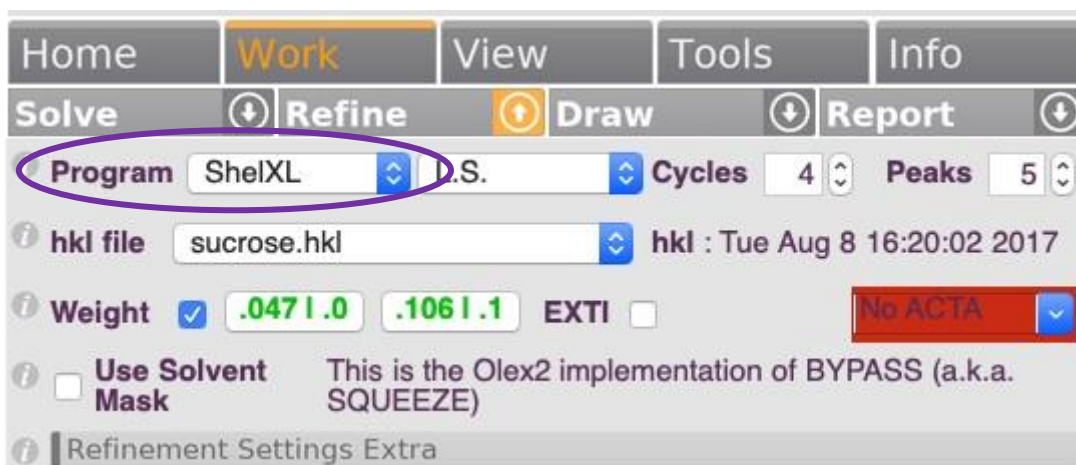
1. Download the Olex2 for macOS DMG file from either:
 - a. (if applicable) Canvas or OneDrive,
 - b. 'imsercdata' server under 'public/Crystallography/Olex2/macOS'. Read more information about connecting to the 'imsercdata' server under 'Data Access' at <http://imserc.northwestern.edu/about-general-faq.html#data>, or
 - c. the Olex2 website (<https://www.olexsys.org/olex2/>). You will need to create an account and download the 64-bit DMG file
2. Install Olex2 by double pressing on the DMG file to make its content available and by dragging the Olex2 folder into your Applications folder. In case you receive a message related to 'untrusted' third party installation software, you need to adjust some security settings:
 - a. Open 'System Preferences' by clicking on the Apple icon and choosing that option
 - b. Select 'Security & Privacy' from the 'System Preferences' window
 - c. Select the 'General' tab and select the lock in the lower left corner to allow changes. Enter your account's username and password, then select 'Unlock'
 - d. In the 'Allow apps downloaded from:' section, select the radio button to the left of 'Anywhere'
 - e. Close the window. You can now install Olex2 into the Applications folder. For security reasons, you may want to repeat this process and check 'Mac App Store' on step #d above
3. The Olex2 icon should appear in the Applications folder and in Launchpad. Press to open Olex2 and the Olex2 GUI should appear
4. If Olex2 prompts you to accept new updates, do this. Look at the bottom of the Olex2 window to check the update progress. Once it is finished updating, close Olex2 and re-open it for the changes to take effect

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B. SHELX SOLUTION AND REFINEMENT PACKAGES

1. Download the SHELX for macOS from either:
 - (if applicable) Canvas or OneDrive,
 - 'imsercdata' server under 'public/Crystallography/SHELX/macOS' (BZ2 files). At minimum, the ShelXT and ShelXS for solutions and ShelXL for refinement files are required. Read more information about connecting to the 'imsercdata' server under 'Data Access' at <http://imserc.northwestern.edu/about-general-faq.html#data>, or
 - Browse to the Shelx website: <https://shelx.uni-goettingen.de/>
 - i. Fill out the registration information to get the download password
 - ii. Follow the links to download the files. Press the 'mac' folder and download the files you would like to use (at minimum, ShelXT and ShelXS for solutions and ShelXL for refinement). Safari will sometimes not download these properly or try to download and unzip them simultaneously which you do not want. We have used google chrome for all the downloads in this guide and it handles all these operations properly
2. Once files downloaded, locate these files in the downloads folder and move them to a temporary folder on the desktop for easy access
3. Unzip these files by double pressing on them
4. Transfer the unzipped files to a folder accessible by Olex2. You have two options for this step depending on your choice of using SHELX through either Olex2 only ([section 4a](#)) or other software packages, e.g., ShelXle ([section 4b](#)):
 - a. [Olex2 only] Copy the unzipped files into the Olex2 package under your application's folder (the folder selected in step A3 for the Olex2 install):
 - i. To see the content of the installed Olex2 package, right press on the Olex2 icon under Applications and select 'Show Package Contents'
 - ii. Navigate to 'Contents/MacOS' and copy the SHELX files there
 - iii. Change the properties of the files we just copied into the 'MacOS' folder. Using terminal, navigate with the '`cd /Applications/olex2-1.5.app/Content/MacOS`' (path might be different on your computer) command into the installation folder and type '`chmod +x shelx*`'
 - iv. Restart Olex2 if it is running
 - v. Olex2 should have the ShelX* options available under the corresponding 'Program' drop-down menus under 'Solve' and 'Refine' (press on the icon with the circled arrow). See example in the figure below

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- b. [Optional when using other software packages] Depending on the security setting of your macOS, you might need to disable macOS' rootless mode otherwise known as the security integrity protocol. This will allow you to write to the '/usr/bin' directory. Alternatively, and easier, if you will be installing Platon (see instructions below), you could use 'usr/local/bin' (when created) instead and skip the following 'rootless' mode directions:
- i. Follow these directions to disable rootless mode:
 - 1st. Shutdown your macOS
 - 2nd. Boot into recovery mode by pressing the power button and then immediately pressing the command and r keys. Hold these keys until the apple logo appears then release. Your computer will now boot into recovery mode. This will take longer than a normal startup
 - 3rd. Open a terminal window by pressing on the utilities tab in the top row and then pressing command line
 - 4th. Type '**csrutil disable**' then press return. There should be a message saying that 'System integrity protocol has been disabled'. You can reenale rootless mode with the command '**csrutil enable**' although leave it disabled for the following steps
 - 5th. Restart your macOS and you will now have rootless mode disabled.
 - ii. With rootless mode disabled:
 - 1st. Open a finder window and in the top row on the screen, press on the 'go' tab and then press 'go to folder'
 - 2nd. Then enter '**/usr/bin**'. This will open the '/usr/bin' folder
 - 3rd. Drag and drop the unzipped ShelX files you downloaded into this folder. This action might prompt you for your computer password. Enter it to complete the file transfer

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- 4th. Open a terminal window
- 5th. From the terminal window, navigate to the folder we just copied the ShelX files into by typing **'cd /usr/bin'** and pressing return
- 6th. If nothing appears to happen, then you have successfully changed directories. If you get a message saying no file or directory exists, check your input and check that you have correctly booted into rootless mode
 - iii. Unpack and change the properties of the files we just copied into the **'/usr/bin'** folder by typing **'chmod a+x shelx*'** add other ShelX executables to this string if you have downloaded them and added them to the **'/usr/bin'** folder
5. Open up Olex2 and check to see if the ShelX programs are available under **'Solve'** and **'Refine'**. If the ShelX programs are not visible close Olex2 and reopen it. Run a refinement and a solution to be sure they work by pressing on the gray tab labeled as **'Refine'** and **'Solve'**. A successful refinement run should give you some numbers for R1 and wR2. A successful solution run should give you some atoms in the main view
6. If you are not installing Platon now (next section):
 - a. Boot into recovery mode as before and open a terminal window.
 - b. Type **'csrutil enable'** then press return. There should be a message saying that **'System integrity protocol has been enabled'**
 - c. Restart your macOS

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C. PLATON

1. Install prerequisite software for compiling and running Platon. Using terminal, install 'Homebrew' by running `'/bin/bash -c "$(curl -fsSL https://raw.githubusercontent.com/Homebrew/install/HEAD/install.sh)"'` without the single quotes ('). It will take several minutes for the installation
2. Install 'gcc' and 'XQuartz' by running `'brew install gcc xquartz'`. In case you already have some of this software installed, this command will update existing versions of 'gcc' and 'XQuartz' to the latest releases which are required if running the pre-compiled version of Platon (see below)
3. Restart your shell or restart your macOS
4. Download Platon for macOS from either:
 - [Compiled version, gcc v11 64-bit] (if applicable) Canvas or OneDrive,
 - [Compiled version, gcc v11 64-bit] 'imsercdata' server under 'public/Crystallography/Platon/macOS'. Read more information about connecting to the 'imsercdata' server under 'Data Access' at <http://imserc.northwestern.edu/about-general-faq.html#data>
 - [Source] 'imsercdata' server under 'public/Crystallography/Platon/Source', or
 - [Latest source] From <http://www.platonsoft.nl/xraysoft/Mac-OSX/platon/> download 'platon.f.gz' and 'xdrv.c.gz'
5. Once files downloaded, locate these files in the downloads folder and move them on the desktop for easy access to a temporary folder called 'platontmp'
6. In a terminal window, navigate to the 'platontmp' folder by typing `'cd ~/Desktop/platontmp'`. Depending on your selection of [Compiled version] or [Source] in [section 4](#), either:
 - [For compiled version] Unzip 'platon-compiled-macOS.zip' by double pressing on the file
 - [For source]
 - i. Unzip 'platon.f.gz' and 'xdrv.c.gz' by typing `'gunzip platon.f.gz'` and then typing `'gunzip xdrv.c.gz'`
 - ii. Compile Platon by typing `'gfortran -o platon platon.f xdrv.c -I/usr/X11R6/include -L/usr/X11R6/lib -lX11'`
Compiling the source is required only when you want to upgrade Platon to the latest version
7. Ensure that the 'platon' file is executable by typing `'chmod +x platon'`
8. Copy the executable file to a location accessible by all software by typing `'cp platon /usr/local/bin'`. This should prompt you for your password and then complete the file transfer. In this step, we are only copying the 'platon' executable file to the '/usr/local/bin' folder and not the entire 'platon' folder. If the terminal

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operation is forbidden, you can open the '/usr/local/bin' folder manually as we did before and drag and drop the 'platon' executable into this folder

- Restart Olex2 if it is running. Platon can be run within Olex2 by pressing on the Platon icon at the top right corner of the Olex2 window. See example in the figure below

Sucrose P2₁
/Users/chris/Library/Application

C₁₂H₂₂O₁₁

a = 7.7727(9)	α = 90°	Z = 2
b = 8.7216(11)	β = 102.983(11)°	Z' = 1
c = 10.8637(11)	γ = 90°	V = 717.63(15)

15.3 R₁ 3.48 %
wR₂ 8.85 %

d min (Mo) 2θ=58.4°	0.73	I/σ(I)	32.7	R _{int}	3.39%	Full 50.5° 96% to 58.4°	99.7
Shift	0.002	Max Peak	0.4	Min Peak	-0.3	GooF	1.046

TWIN LAW (-1.0, 0.0, 0.0, 0.0, -1.0, 0.0, 0.0, 0.0, -1.0), BASF [0.9(10)]
Structure sucrose loaded

- If Platon works, you do not need the files in the '~/Desktop/platontmp' folder anymore and it is safe to delete that folder from your desktop

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REVISIONS

V1.03 2022/1/12	<ul style="list-style-type: none">• Modification of the Platon installation section for Windows
v1.02 2021/12/31	<ul style="list-style-type: none">• Updated for Olex2 1.5• Modification of the Platon installation section for macOS• macOS instructions have been tested on macOS 12.x (Monterey), macOS 11.x (Big Sir), and macOS 10.15.x (Catalina)
v1.01 2021/1/8	<ul style="list-style-type: none">• Instructions updated for macOS sections due to the 64bit nature of macOS 10.15.x (Catalina) and macOS 11.x (Big Sir)• 'XPREP' section removed since only a 32bit version of the software was available and it was found to be incompatible with 64bit-only macOS operating systems. Windows users are not affected
v1.00 2020/1/7	<ul style="list-style-type: none">• Release of original version of the user manual. Special thanks to James Passarelli for working on the macOS installation sections for all software ('Olex2', 'Platon', and 'XPREP')
