Notes from the Chat on May 19, 2020

For reference, the most recent course materials are here:
https://xtallography.ca/index.php/xtal/meetings/cccw20/program/

pointer > right click and select pointer

space bar = next

or "n" = next

It might be worth pointing out that a "full set" of data means all of the data in the asymmetric part of the diffraction pattern has been collected rather than a full sphere

“Full set” depends on symmetry

https://dictionary.iucr.org/Main_Page

Cu is ~2x the wavelength [of Mo], so the pattern is expanded over a much larger area, and depending on the size of the detector may take many more scans to get a complete data set

[In OLEX2] clicking on the orange box in the upper right corner will reset the zoom

[setting the right click on the Mac] Click on the Apple symbol > System Preferences > Trackpad. There you can set the “zoom” function. It should be two fingers.

[In OLEX2] There are sliders to hide/show Q peaks if the touchpad isn't working.

type "legend" to see the legend. Type legend again to hide it.

This is a "cheat sheet" that Amy and her colleague produced for some of these commands:
http://xtallography.ca/wp-content/uploads/2018/05/Olex2-Cheat-Sheet.pdf

These are Ilia's notes: http://xray.chem.wisc.edu/Resources/Manuals/Ilia_Guzei_notes_on_OLEX2.pdf

"telph" will show the isotropic displacements of the hydrogen atoms.

Is there a way to highlight double bonding? In my experience, double bonds are discerned from bond length, and sometimes you find Q peaks where the pi electrons are

Control-T toggles text [in OLEX2] and lines ## determines the number of lines you see.

Lines -1 fills the screen.

You can modify the way bonds are displayed. Right click on a bond, Graphics->Primitives, and then check what you want - double bottom cone and double top cone and uncheck other boxes

Pencil w/o the blue works for editing on mac the only thing to remember is that it always opens the instruction files (.ins). Going to the directory and using a text editor works on every file

The command "shell" will open the default shell on your OS in the working folder.

To change the size of the right-hand gui in OLEX2 type ‘skin ###’. You can always go back to the default sizing by typing: skin 500

Was the geometry tab with the plane to plane interactions an extension the standard OLEX2 download lacks? No; go to View --> Geometry

OLEX2 considers Q peaks part of the structure, so when they are displayed the molecules are different and would not "match" for overlay purposes. The molecule composition must be exactly the same too. Please try hiding the H atoms and then trying to match

ctrl-H has three position: 1. Hide H atoms; 2. Show H atoms; 3. Show H atoms with hydrogen bonds.

if you type "move" the molecules will be repositioned closer to the center of the cell

Go to Naming, fill in start & Type and then hit Name. It will give you a tiny circle that you use to click on the atoms you want

Don't select an atom yet. Leave everything unselected. In the Naming panel pick a start number and atom type, click on the Name button and the cursor will change. Then click on the atom, but - make sure the little dot in the cursor is over the atom you want to rename.

for those still around and willing to answer questions: what is the difference between the “move” command and the button in the top rightmost corner (circle with arrows)

The button assembles fragments.

There are alternate options for moving molecules to symmetry equivalent positions.

View --> Symmetry Generation --> Symmetry Tools

You will see that there are Move Near, Centre on Cell.

Adjacent to these you will see a "i" button.

If you click on "i" it will tell you how each "move" works.

support@olex2.org. Horst Puschmann is very, very helpful, so if we can't get you sorted out, he will.

11.00000 means: (1.000) + (10) = 100% of the time, and fixed at that value

http://shelx.uni-goettingen.de/shelxl_html.php

In OLEX2 if you would like to generate hydrogen bonds you can type HTAB at the command line.

"HTAB -t=Br,I", etc...will generate non-classical H-bonds (just specify one type of acceptor at a time).

You can vary your D...A distance, and D-H...A angle by typing HTAB 3.5 140 (for example; you can change the length and angle for your purposes).

https://journals.iucr.org/j/issues/2008/01/00/ks5161/index.html