OIM Primer 2020:
Style guides, Software Tutorials, and Laboratory Best Practices

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OIM Primer
Fall 2020

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1 Microsoft Office

Point People: Tawney Knecht (tknecht@uoregon.edu) and Grace Lindquist (glindqui@uoregon.edu)

1.1 Homework and In-Class Assignments

Before class (due at the start of the workshop):
- Download Microsoft Office
- In Excel:
  - You will be provided an Excel file containing FTIR data on Canvas. Create a scatter plot of this data set in Excel, following the tutorial in section 1.4. You do not need to change the settings of the graph to look nice yet as we will do this in class; just make a graph.
  - Save the file and be prepared to edit in class.

In class:
- Make a presentation-ready graph of the provided data following the primer below (section 1.4).
- Save the graph template
- Paste your graph into a Microsoft PowerPoint slide.

Homework (due at the start of the following week):
- A single PowerPoint slide (*.pptx) with an appropriately-sized graph.
  - Include slide number and an assertive title (example of good and bad title is found in the PowerPoint primer, section 1.3)
- Follow this format for your file submission: LastName_FirstName_Graph.pptx.

1.2 Download Instructions

Go to the following website: https://software.uoregon.edu/
Log in with your DuckID

Welcome to the UO Software Download Center!

Login with your DuckID to access your available software
Navigate to the Software Center (left menu):

Input the system you are using:

Click on either “Microsoft Office 2016 for Windows/Mac” or “Microsoft Office 365”:

Click on “Obtaining Software” link and follow instructions.

1.3 Basics of Microsoft PowerPoint

You will give many presentations over your graduate career, and PowerPoint is the preferred presentation software. This primer is not meant to be an extensive overview of PowerPoint, but rather a list of tips that may be helpful in making presentations.

1.3.1 General Presentation Guidelines

This guide will provide several general tips for good presentations, but please note that you should ALWAYS defer to your PI's preferences for making a good presentation. Remember, the goal is to communicate your science effectively to your audience.

In general, follow these rules:

- Sans serif fonts (Arial is a generally accepted font choice)
- Main text font sizes no smaller than 16 pt
- Minimal text on slides
  - Any text should help the audience follow the presentation, not distract them from what you are saying
  - Bullet points are often more helpful than full sentences
- No dark backgrounds
- No unnecessary or distracting graphics
- Slide numbers in bottom right corner (always include slide numbers)
  - To insert, go to the Insert tab and click on the icon in the Text section of the toolbar
  - Check “Slide Number” and click “Apply to All”
- Slide titles should be assertions and highlight the conclusion of the slide
  - Example of bad title: FTIR Data
  - Example of good title: FTIR data indicate monomer is consumed during reaction

1.3.2 Slide Master

Slide Master is a way for you to create a template of a presentation design that you can apply to future presentations to save you time. In this, you can select fonts, font sizes, change placement of text boxes, and create simple but professional designs.

To start, go to the View tab and click “Slide Master”

Under Fonts, choose your preferred font (Arial will be used in this guide)

In the second slide, arrange textboxes so they fill the space appropriately, and change the font sizes if necessary.
If desired, add simple design features. Common examples include colored boxes at the bottom in which to put references, or a line at the top to separate the title from the rest of the slide. Examples are shown below, created using the box and line shapes (a section on shapes is below). Be careful to not overdo this step and be open to feedback from PIs and other students if they feel the design features are unnecessary and/or distracting.

To save the theme to apply to future presentations, go to the **Slide Master** tab, click on "Themes" dropdown and click "Save Current Theme."

Save in the desired folder. To access this theme later, open a new presentation, go to the **Design** tab, and click through the themes. The theme you saved should appear in this list.
1.3.3 Shapes

To insert a shape, go to the Insert tab, click on the “Shapes” dropdown and select the shape you want to draw.

Once a shape is drawn, you can edit the fill color (“Shape Fill”) and outline color and thickness (“Shape Outline”) in the Format tab.

Use the “Align” dropdown in the Format tab to align shapes in an aesthetically pleasing manner.
Helpful tips for drawing shapes:

- Notice that lines will appear in PowerPoint when you move shapes around to help you align them in an aesthetically pleasing manner
- Select multiple shapes by either clicking and dragging your cursor to form a box around them, or by pressing CTRL while clicking on multiple shapes
- Group shapes by selecting multiple shapes, right clicking, and selecting “Group.” Shortcut: CTRL+G
- Move shapes or groups of shapes to the front or back by right clicking on shapes and selecting one of the following:
  - Move to front
  - Move to back
  - Move forward
  - Move backward
- Holding SHIFT while drawing a line/arrow will keep the arrow perfectly horizontal or vertical as you draw it
- Holding SHIFT while scaling a shape will lock its aspect ratio
- Holding SHIFT while moving a shape will restrict the movement to only the horizontal and vertical directions (helpful for alignment of multiple shapes)
- Holding CTRL while moving a shape will duplicate that shape
- Holding SHIFT while you rotate a shape will rotate it by 15° at a time

1.3.4 Animations

Animating in textboxes, shapes, and/or figures can be helpful in presentations to prevent too much information being presented all at once. To animate in an object, select the object, go to the Animations tab, and select “Appear.” Do not use distracting animations.

You can also make objects disappear by selecting “Disappear” under the same dropdown.

To manage animations, click on “Animation Pane”
1.4 Basics of Microsoft Excel

There is a myriad of resources online to help with Excel, so this guide will only point out a few helpful tips that you may commonly use.

1.4.1 Inserting Data

Several data sets already come as Excel files, others may come as .csv files. To insert from a .csv file, hit **CTRL+A** in the .csv file to select all of the data, hit **CTRL+C** to copy, go into Excel and select a cell and then hit **CTRL+V** to paste.

1.4.2 Text to Columns

Often, pasting data from a .csv file pastes all of the data into a single cell. To separate numbers into different cells, go to the **Data** tab and click “Text to Columns.”
A window will appear. Depending on the data format, you will select “Delimited” if data are separated by commas, spaces, or tabs, and you will select “Fixed width” if data are aligned. “Delimited” is more common. Click “Next.”

Select your delimiters and check the Data Preview to ensure the data are separated the way you need, then click “Finish.”

1.4.3 Highlighting Data

To highlight data, simply click and drag over the data you need. For large data sets, you can also hit **CTRL+SHIFT+Arrow Key [←↑→↓]** to highlight data to the end of the data set in the direction of the arrow you pressed.
1.4.4 Inserting Formulas

A good resource if you are new to formulas is here:
https://corporatefinanceinstitute.com/resources/excel/study/basic-excel-formulas-beginners/

The general format of a formula is “=Operation(Cell#:Cell#)”

For example, if I want to add numbers in cells A1 through A10, the formula would be “=SUM(A1:A10)”

Common formulas:
- Addition: =SUM(data range)
- Average: =AVERAGE(data range)
- Standard Deviation: =STDEV(data range)
- Minimum: =MIN(data range)
- Maximum: =MAX(data range)
- Division (for example, cell A1 divided by A2): =A1/A2
- Multiplication (for example, cell A1 times A2): =A1*A2

To select the data range, either drag over the desired data when prompted, highlight the data as discussed previously, or manually type in the data range.

1.4.5 Making a Graph

Please see section 3.3 in the Igor Pro tutorial for elements of a good graph. Many groups may prefer you use other software to make graphs, but Excel is a good starting point, and it is possible to make professional-looking graphs in Excel. Please defer to your mentors and PIs’ expectations for making graphs, the following is only meant to show you the features that can be used in Excel.

For an example, the following data will be used to make a graph:

<p>| | | |</p>
<table>
<thead>
<tr>
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<tbody>
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<td>9</td>
<td>9</td>
<td>18</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>20</td>
</tr>
</tbody>
</table>

To make a graph, first determine what type of graph you need (scatter, line, bar, etc.). For this example, a scatter plot will be used. Select the graph type from the insert tab in the “Charts” section.
A blank graph will appear. Right click on the graph and select “Select Data.” A new window will pop up. Click **Add**.

A new window will pop up where you can name your data (useful when graphing multiple data sets) and select the X and Y values of the data set. Here, I will plot Sample 1 with X values as A1:A10 and Y values as B1:B10. I will then plot Sample 2 with X values as A1:A10 and Y values as C1:C10. To select X values, click on the ▲.
next to the “Series X values:” line, then highlight the desired data. Do the same for the Y values. Hit OK on all windows.

The graph should now look like this:

Delete gridlines by clicking on the gridlines and hitting “Delete” on your keyboard.
Add axis titles by selecting the green plus sign at the top right of the graph when you click on the graph. Select “Axis Titles.”

Edit the axis titles by simply clicking on them and typing. You can adjust the color, font, and font size by operating in the **Home** tab. You can also do this for the axis numbers by clicking on those numbers. In this example, axis titles were changed to Arial 14, black and axis numbers changed to Arial 12, black.
Edit the axes by first clicking on the axis numbers (this example will start with the X-axis). A menu should pop up to the right of the screen. In this window you can change the axis range, among other features. Play around to see what each item does. In this example, X-axis range was changed to have a minimum of 0, maximum of 10, major unit as 2.0, and the Y-axis range was changed to have a minimum of 0, maximum of 20, major unit as 5.0. Under “Tick Marks” the major tick marks were selected to be outside.

With the axis still selected, click on the paint bucket to change the thickness and color of the line. In this example, lines were selected to be black with a thickness of 1.5.
To close the axes, click on the chart area such that just the chart area inside the axes (not the whole chart) is selected. On the right, the “Format Plot Area” menu should appear. Under “Border” select “Solid line” and change the settings. In this example the border was chosen to be black with a thickness of 1.5.

To add lines of fit, select a point in the data set, right click, and select “Add Trendline.”
In the “Format Trendline” menu on the right, scroll to the bottom and check the boxes next to “Display Equation on chart” and “Display R-squared value on chart.”

Edit the text font by clicking on the equation and editing using the **Home** tab. In this example, it was changed to Arial 14.
This guide did not go through all of the features in the formatting menu that appears when you double click on the chart or axes. Please click through all of the menu items to see what can be edited, and how they affect the chart. If you have questions about how to edit something, please first search for help online and then contact Tawney if you need additional help.

1.4.6 Saving and Applying Chart Templates

Now that you’ve created a professional-looking chart, you can save these settings and apply them to future graphs to save some time and keep your graphs consistent.


To save a template, follow these steps:

1. Make a chart with all of the desired formatting features (please defer to your mentors’ and PI’s preferences)

2. Right click on the chart and select “Save as Template…”
3. Save template file in the default folder as desired file name.

To apply templates, follow these steps:

1. Make a new chart

2. Right click on the chart and select “Change Chart Type…”

3. A window will appear. Select “Templates” from the left column and select the desired template. Hit OK.
4. Note that this will not affect the size of your chart. For consistency, resize your chart using the **Format** tab and entering the desired height and width of your chart. 4” height and 4.8” width are good starting points, but again, defer to your PI’s and mentors’ preferences.
2 MestReNova

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NMR Facilities Director: Nanette Jarenwattananon (njaren@uoregon.edu)

2.1 Homework and In-Class Assignments

Before class (due at the start of the workshop):
- Follow Download Instructions for MestReNova (detailed below).
- Follow Steps 1-2 of the MestReNova primer below (open the provided raw data file in MestReNova).

In class:
- Follow Steps 3-7 in the MestReNova Primer below.

Homework (due at the start of the following week):
- A MestReNova file (*.mnova) with the proper settings and a worked up $^1H$ NMR spectrum for the data file provided (1-allylnapthalene). Follow this format for your file submission: LastName_FirstName_Mnova_HW.mnova.
- A single PowerPoint slide (*.pptx) with an annotated NMR spectrum for the provided data file and compound (see Step 6 for what this should generally look like). Follow this format for your file submission: LastName_FirstName_Mnova_HW.pptx.

2.2 Download Instructions

1. Go to http://hotwax.uoregon.edu/mnova
2. Read the PDF installation guidelines: http://hotwax.uoregon.edu/mnova/MestReNova_Installation_Instructions.pdf (this should fix 99% of problems that come up during installation of MestReNova)
3. Follow instructions for downloading and installing MestReNova
2.3 Using MestReNova

**STEP 1**

Once you get licenses and software installed, open MestReNova. You should see a blank page. If you don’t have the “Pages” window, go to View → Pages.
STEP 2
Open a file in MestReNova. Go to File → Open → Click and drag the folder from your experiment into MestReNova.

STEP 2, continued
You should see a spectra. Now we need to set up your preferences to make your spectra more readable!
STEP 3
Once you have a spectrum open, we can set up your preferences to make your spectra more readable!
1. Click on the spectra so that the green boxes around the edges/corners show up.
2. Right click and choose “Properties”
3. This is where the majority of your NMR aesthetics will be modified.

STEP 3, continued
Under “General”
1. If you want to see the file name of your NMR while looking at the spectra, make sure the “Title” box is checked (green highlighting)
2. Go to Font → Select Font → Choose Arial, Regular, 12 pt font (this will be the standard font for all text in MestReNova)
**STEP 3, continued**
Under “Grid”
1. Uncheck ALL the boxes

**STEP 3, continued**
Under “1D”
1. You can change the color of the actual spectra here. I prefer to use black most of the time.
2. Line width can be increased. This will help with visibility, especially for presentations. Line width ≥4.0 is recommended.
**STEP 3, continued**
Under "Scales"
1. Go to Font → Set to Arial, Regular and 12 or 14 pt font (I prefer 14 pt)

**STEP 3, continued**
Under "Scales" → "Horizontal"
1. Change the "Label" box to say "$\delta$ ($\mu$S)"
**STEP 3, continued**
Under “Scales” → “Vertical”
1. Uncheck the small box next to “Vertical”

---

**STEP 3, continued**
Under “Peaks”
1. Click on “Font” and change to Arial, Regular, size 12 or 14 pt
**STEP 3, continued**

Under "Integrals"

1. Click on the dropdown menu for "Font" and choose “Select Font.” Change your font to Arial, Regular, size 12 or 14 pt
2. Uncheck the small box next to “Curve”

**STEP 3, continued**

I don’t change any other settings under "Multiplets," "Fitting," "Assignments," or "Prediction."

The last two steps are to click “Apply” on the bottom right and then “Set as Default” on the bottom left so every spectra you open after this will open with these settings!
STEP 4
There are a few steps you should take to process every raw data file. Use the following shortcuts to process the data file:
1. “b” will open a window for “Baseline Correction.” Choose “Whittaker Smoother” from the dropdown menu and hit OK (left image below)
2. “w” will open a window for “Apodization along t1.” Check the box for “Exponential” and change the value to 1. Hit OK (middle image below)
3. “I” (lowercase L) will change your curse to set your reference peak. You always need to reference your spectra appropriately before comparing chemical shifts. Once you hit “I” move your cursor over the appropriate peak and click. Change the value to the appropriate chemical shift (in the example, I am setting the peak at ~0 to exactly 0.00 for tetramethylsilane). If you want to label the peak, you can type a label into the “Annotation” text box. Hit OK (right image below)

STEP 5
Zooming, picking peaks and integrating.
1. Hitting “z” toggles through different types of zooming. You usually will want to be on the left to right zoom (red bar will be horizontal). Zoom in enough that you can clearly see splitting.
2. Command+k (or ctrl+k for windows) will help you pick peaks. Click on a peak to label its chemical shift. (left image below)
3. “i” will allow you to integrate peaks. Click and drag across the distance you want to integrate. The integral value will show up below the spectrum.

Picking peaks

Integrating peaks
**STEP 6**
Adjust integral values. You want integral values to reflect the actual molecule. For the example below, the two doublets you see correspond to the aryl protons of para-CF₃-allylbenzene and thus should both integrate to 2. To adjust integral values, hover over the horizontal integration bar and right click, choosing “Edit integral.” Change the value for “Normalized” to the appropriate number of protons in your molecule (in this case, 2). Hit enter.

**STEP 6, continued**
After normalizing one integral, all integral values automatically adjust and should reflect the relevant molecule.
STEP 7
Presenting your NMR data.

NMR spectra
- Properly labelled with the structure
- Solvents and impurities labelled
- Important area emphasized
- Fonts are ≥12 pt

STEP 7, side note
If you are working with a molecule that has more than one NMR-active nuclei, you should get spectra of all relevant nuclei.
2.4 Other Notes and Tips

- Always compare product NMR spectra to starting material spectra
- Think about which peaks you expect to disappear/appear/shift going from starting material to product
- Check the “Common $^1$H NMR impurities” list to see if impurities are from solvents that you used during the reaction (or during work-up!)
- Pay attention to splitting when assigning peaks (i.e. if a proton has two neighboring protons, it should be a triplet)
- Remember that you need to take NMR spectra in the same solvent to compare chemical shifts (i.e. if you have an NMR spectra of your starting material in CDCl$_3$, you should take an NMR spectra of your product also in CDCl$_3$) unless solubility prevents this
- The AIST structural database has NMR spectral data for a wide range of common starting materials (https://s dbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi)

2.5 Supplementary Resources

- Alternative MestReNova tutorial: https://www2.chem.wisc.edu/~cic/nmr/Guides/Other/Mnova_NMR_Training_for_chemists_on_1D_and_2D_NMR-Version_8.0.pdf
- Common NMR chemical shifts ($^1$H, $^{13}$C, $^{19}$F, $^{31}$P, $^{77}$Se) organized by functional group: https://organicchemistrydata.org/hansreich/resources/nmr/?index=nmr_index%2F1H_shift
- Common $^1$H NMR impurities (list of chemical shifts for solvents/common impurities for most relevant NMR solvents): https://pubs.acs.org/doi/pdf/10.1021/om100106e
3 ChemDraw

Point Person: Kiana Kawamura (kkawamu2@uoregon.edu)

3.1 Homework and In-Class Assignments

Before class (due at the start of the workshop):
- Follow Steps 0-2 in the ChemDraw Primer below (downloading ChemDraw software and initial set up).
- Draw the following reaction scheme in ChemDraw. We will work on editing the individual structures and overall reaction during the in-class workshop.

Before class reaction scheme:

\[
\text{PhOH} + \text{BrCH}_2\text{CH}_2\text{Br} \xrightarrow{\text{K}_2\text{CO}_3, \text{acetone, reflux, } 8\text{ h}} \text{PhOCH=CH}_2
\]

- OPTIONAL: If you want a challenge, you can work on making the following organometallic synthesis reaction scheme.

Organometallic synthesis reaction scheme:

\[
2\text{CH}_2\text{MgCl} + \text{NiCl}_2(\text{anhyd}) \xrightarrow{\text{THF, } 50\ ^\circ\text{C, } 4\text{ h}} \text{dippNiN}_2\text{N}_2\text{dipp}
\]

In class:
- Follow Steps 3-8 in the ChemDraw Primer below.

Homework (due at the start of the following week):
- A ChemDraw file (*.cdx) with the proper settings and one example reaction drawn out (can be an example from class or one from your rotation). Follow this format for your file submission: LastName_FirstName_ChemDraw_HW.cdx.
3.2 Download Instructions

**STEP 0**
Get the ChemDraw software
1. Go to [https://researchguides.uoregon.edu/chemistry/software](https://researchguides.uoregon.edu/chemistry/software)
2. Follow instructions to download and install ChemDraw AND the necessary licenses

<table>
<thead>
<tr>
<th>Chemdraw</th>
<th>Mac and Windows</th>
</tr>
</thead>
<tbody>
<tr>
<td>- The Library’s license requires yearly updates, which means some action is required to keep the software running after each cycle (generally in Fall term). Scroll to the Oregon section of this download page. - Use the second link to set up your account and the first link to refresh annually.</td>
<td>Available on compounds in the Libraries</td>
</tr>
</tbody>
</table>

3. You will want to **Register** with Perkins Elmer and will need to make an account.
3.3 Using ChemDraw

**STEP 1**
Get to a good starting point in structure aesthetics.

File ➔ Apply Document Settings from ➔ ACS Document 1996

**STEP 2**
Get all the tool bars open that you will need.

From the “View” dropdown menu, check the following:
- Show Crosshair
- Show Rulers
- Show General Toolbar
- Show Style Toolbar

Note: These are my personal preferences. I also use “Show Analysis Window” often. If you want other toolbars open constantly, feel free to keep them open by clicking on them.

Explanation
This setting is a good starting point. It increases the font size to bond length ratio to make your structures more readable.

Default settings ACS 1996
**STEP 3a**
Expand the space you have to work with

File → Document Settings → Layout

I never make my ChemDraw sheet wider, only taller, which makes it easier to keep track of everything, in my opinion. I suggest either choosing Document Type → Poster and increasing the height as needed or choosing Document Type → Pages and increasing the number of rows.

**STEP 3b**
Increase the clarity of your bonds.

File → Document Settings → Drawing

Making bonds thicker will make them more clear and easier to read. See below for a comparison of default settings to my preferred line width of 0.015 in.

ACS 1996
Default line width = 0.0084 in

Modified settings
Increased line width to 0.015 in
**STEP 3c**
Make your fonts consistent.

File → Document Settings → Text Captions/Atom Labels

I prefer to use Arial. You can use a different font, but best practice is to use a Sans Serif font.

**STEP 4**
Being consistent.

File → Duplicate

A new document will pop up. Edit the name and proceed from there. You can delete all the contents to have a “fresh” document. This is the easiest way to make sure these settings stay constant for all the ChemDraw structures and schemes you make.
**STEP 5**
Drawing aesthetically pleasing structures!

Bond angles are important. When working with simple organic molecules, using Structure → Clean Up Structure can be incredibly helpful! Make sure to highlight the structure that you want to “clean up.”

**STEP 6**
Drawing aesthetically pleasing reactions!

Aligning and spacing things out in a reaction scheme is critical for making reaction schemes easy to read. Highlight all the pieces of a reaction and use Structure → Clean Up Reaction to get all the pieces of a reaction to space out and align correctly.

Note: ChemDraw is a little picky and you need the text above and below the arrow to be separate text boxes to use the “Clean Up Reaction” function.
**STEP 6** – a closer look

![Chemical diagram]

- Text/reagents are properly subscripted
- There is a space between numbers and units
- Reagents and arrow are aligned vertically
- All the text and the reaction arrow are aligned in the center
- A superscript 0 or 0 is used (do not use a subscript 0 or 0)
- Spacing between reagents and arrow and product is the same

*Note: All information relevant to the reaction conditions are included* (reagents, solvent, temperature, time, etc.). The numbering implies that these were separate steps in the reaction set-up/progression. If everything is one pot, numbers are not used usually.

**STEP 7**

If "Reaction Clean Up" isn't working, you can use the "alignment" and "distribute" functionalities under the "Object" menu to manually clean up reaction schemes.
STEP 8
Putting ChemDraws into PowerPoint.
1. In ChemDraw, highlight what you want to copy to PowerPoint. Use Command+c or control+c to copy.
2. In PowerPoint, use command+v or control+v to copy onto your slide.
3. Right click on the image and select “Size and Position” to open the “Format Picture” window.
4. Make sure “Lock aspect ratio” and “Relative to original picture size” are checked.
5. **Scale ALL your ChemDraw structures to the SAME “Scale height/Width”**
   1. Using the example below, that means every single ChemDraw image should be scaled to 250% throughout the entire presentation.

Supplemental Information
General organometallic complexes in ChemDraw

ChemDraw is pretty good at making good organic molecules, however, it struggles with the geometries and spacing of organometallic complexes. This means manual adjustment is almost always needed.

Making complexes with coordinating alkenes

1. Draw the fragments
2. Orient the fragments around metal center
3. Draw bonds from metal center towards alkene
4. Use arrow keys to move things around until oriented well
5. Bring alkene to front so bond from metal doesn’t overlap (highlighted in yellow)
Supplemental Information
Making catalytic cycles in ChemDraw

1. Sketch out the intermediates you will need so you know the general spacing of your cycle.

2. Draw a circle the approx. size of your cycle and orient all the metal centers on the circle.

3. Add arrows and adjust curvature to fit the circle. Add reagents entering or leaving the catalytic cycle.

4. Use arcs for reagents entering cycle and arrows for products leaving cycle. Delete the guiding circle and you’re done!
4 Igor Pro

Point Person: Tawney Knecht (tknecht@uoregon.edu)

4.1 Download Instructions

- Go to the following website:
  
  https://www.wavemetrics.com/order/order_igordownloads.htm

- Click on either Igor8.dmg (for Macs) or setupIgor8.exe (for Windows)
- Follow the prompts to install Igor
- Use the following license information when prompted:

  Serial number: 80120
  Activation key: NGNA-DJZM-ASVP-UJMZ-KSSS-UNDE-ZPP
4.2 Elements of a good graph

A good graph has the following features:

- Data is appropriately represented in accordance with the literature (i.e. use example plots from the literature to guide your graphing)
- Data fill the space that is given
- Data are easy to interpret
  
  For example, if you have multiple traces on the same graph, either color-code them and ensure the colors are different enough to be able to easily distinguish or use markers to denote the different traces. Keep in mind color contrast for color-blind folks.
- Axes are properly labelled, with units
- Text is large enough to read
- Axes use scientific notation, where appropriate
- No distracting/unnecessary information or graphics
- Aesthetically pleasing (use the literature and examples to guide this)
  - No gridlines
  - Proper aspect ratio
  - Mirrored axes
  - Lots of other components that will come with time and practice…

Example of a bad graph:

Example of a good graph using the same data, plotted in Igor Pro:
4.3 How to Make a Graph in Igor Pro

4.3.1 Pasting data into Igor Pro from Excel

You can paste data directly into Igor from most files, but it is generally easier to start in Microsoft Excel, and then copy and paste from there. With your data in Excel, first create a unique label for each column. Note that Igor will not allow you to paste in more than one column with the same name, so make sure each column has its own label. To create a row above the data in Excel, highlight the top row, right click and select “Insert.” Then create unique labels for each column. In the example data, there are two sets of IR data, with the first two columns being the y-values (absorbance) and the third column being the x-values (wavenumber). I have chosen to label them as shown below:

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Y_A</td>
<td>Y_B</td>
<td>X_WIN</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>-15.3183</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>-15.2973</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>0</td>
<td>-15.2763</td>
</tr>
</tbody>
</table>

Next, select all of your data in Excel either by clicking CTRL+A to select all, or highlight the top row of data (including the titles) and clicking CTRL+SHIFT+↓.

Once desired data is selected, click CTRL + C to copy the data, go into Igor, select the top left box in the table, and click CTRL + V to paste the data. The table should look like this:
4.3.2 Creating a Graph

To do this, go to the Windows tab and select “New Graph…” A window will pop up (shown below).

In the **XWave** column, select your desired X-values. In the **YWave(s)** column, select your desired Y-values. You can select multiple (if they have the same X-values) by holding down CTRL as you click on them.

Hit **Add** in the top center of the window, and then click **Do It** at the bottom left. You should then have a graph that looks like this:
4.3.3 Editing the Graph

Disclaimer: this guide will walk you through how to edit all of the features of a graph. The goal of this guide is not to show you how to make a graph look a specific way, just to show you how to edit all of the features, so please defer to your mentors and PIs for what constitutes an acceptable graph for presentations/publications.

To edit the graph, double click on one of the axes. A window will pop up with all of the parameters you can change to edit the graph. This guide will go through all of the tabs in the following instructions. As you change settings in this window, watch how it affects your graph.

4.3.3.1 Axis

In the first tab, you can change the appearance of your axes. In the top left, you select which axes you are affecting (x, y, or both). In the image above, it says “Multiple Selection…” because both axes are selected.

The **Mode** section is where you can change your axis to a log scale, which is useful in many situations, but not for this example.

The **Axis** section is where you change the appearance of your axes. For this example, I unchecked the “Axis standoff” box, selected “No ticks” from the **Mirror Axis** dropdown, and changed “Axis Thick” to 2.

The **Font** section is where you change the axis label and title color, size, and font. The default is Arial, which I left unchanged. I changed the size to 20 and left the colors black.
4.3.3.2 Auto/Man Ticks

Here is where you change roughly how many numbers you want on your graph, as well as how many ticks. In the **Automatic Ticks** section, I changed the ticks to be approximately 5, and I checked the “Minor Ticks” and changed the “Minimum Sep” to 10. These are good values with which to start, but these numbers will depend on the specific data. Play around with different values to see how these numbers affect your graph. Also note that you may need to change these for each individual axis, in which case you need to change which axis you are affecting by selecting the appropriate axis from the **Axis** dropdown menu in the top left corner of the window.

4.3.3.3 Ticks and Grids

These settings rarely need to be changed. In the **Exponential labels** section, you can change from “Engineering” to “Scientific,” and you can determine how many decimal places are included by changing the high trip and the low trip. For this set of data, the default values work well.
In the **Tick Dimensions** section, you can change whether the ticks are on the inside or outside, and you can change the length and thickness of the ticks. In this example, I left the location on “Outside” and left the rest as “Auto.”

### 4.3.3.4 Tick Options

These settings rarely need to be changed, but this is where you can change how much of your axis contains ticks. Generally, ticks will span the entire length of the axis, so you will keep the “Enable ticks between” to -infinity and infinity.

### 4.3.3.5 Axis Label
Select your font and font size. Once you change anything, code will appear in the Axis Label box. Note that this code will affect anything after, but not before, the code. When selecting a font size, \Z## will appear. So to change the font to 20, \Z20 appears in the box, and a preview is shown below it.

For superscript or subscripts, select which you want from the “Special” dropdown menu. For subscripts, \B will appear. For superscripts, \S will appear. After you type your sub/superscript, exit out by selecting “normal” from the “Special” dropdown menu and \M will appear. Again, select the font size you want and finish typing your title and units. Examples are shown in the images above. You can also change the style (bold or italics) as well as the text color from the “Special” dropdown menu and insert special characters or symbols. Explore this on your own to see what the “Special” dropdown offers.

As a shortcut, you can also type the code directly into the Axis Label box. Some common codes are listed below (case-sensitive):

- \Z[insert font size] = changing the font size
- \S = superscript
- \B = subscript
- \M = normal (i.e. exit out of sub/superscript)
- \f00 = no style (i.e. exit out of bold or italics)
- \f01 = bold
- \f02 = italics
- \f03 = bold and italics
- \JC = justify center
- \JL = justify left
- \JR = justify right
4.3.3.6 Label Options

These settings rarely need to be changed. Here you can change the rotation of your axis title, as well as the axis labels themselves.

4.3.3.7 Axis Range
Change your axis range to be something appropriate. In the **Autoscale Settings**, this is where you can reverse your axis if necessary (not necessary for this data set). You can also select “Round to nice values” from the first dropdown, or you can manually set your axis limits in the **Manual Range Settings** box. The settings I chose for this data set are shown in the figures above.

Hit **Do It**. If you’ve changed all of your settings to this example, the graph should look like this:

4.3.4 Editing the Traces

To edit the traces, double click on one of the traces and you should get the following window:
Select which trace you want to affect in the **Trace** box. Then you can change several features such as the line size, the line style, and the color. You can also offset traces by checking the “Offset” box and typing in how much you want to offset x and y. Additionally, this is where you can change the **Mode**, which is generally “Lines between points” or “Markers.” This depends on the specific data set, as well as how that data is generally plotted. Defer to your mentors, PIs, and the literature for guidance on this.

For this example, I changed the line size to 2.00 for both traces and changed the Y_A trace to be black and the Y_B trace to be maroon. Use colors you feel are appropriate. Hit **Do It**.

### 4.3.5 Changing the Graph Size

Double click on white space in the graph window, but outside of the actual graph. You should get the following window:

This is a matter of what aspect ratio looks best for your data, as well as personal preference. I changed the Width mode to Aspect and changed it to 1.2*height.
then changed the Height mode to “Absolute” and chose 4 (inches). Play around with these settings to see how each affect your graph.

Hit **Do It**. If you’re following along, your graph should look like this:

![Graph](image)

### 4.3.6 Adding Annotations

To add annotations, either a legend or text, right click on the graph and select “Add Annotation…”. You will get the following window:

![Annotation Window](image)

To simply add text, type in the **Annotation** box. The same codes as previously discussed related to font size, sub/superscripts, etc. apply here.

To make a legend, select “Legend” from the **Annotation** dropdown menu in the top left corner, and you will get the following window:
Edit the labels as well as the font size. I labeled mine as “Sample A” and “Sample B” with a font size of 20, as shown below:

NOTE: many PIs prefer you not use legends, but instead label the data directly. Please defer to PI preferences when making graphs.

In the **Frame** tab, you can put a box around your annotation, change the background color, and more. Play around with these settings to see what they do.

In the **Position** tab, you can rotate the annotation. Again, play around with the settings to see what they do.

### 4.3.7 Duplicating the Graph

To duplicate the graph, select the **Edit** tab from the top of the Igor window and select “Duplicate Window.” Note that you can also click CTRL+D as a shortcut.
4.3.8 Saving Graphics

To save graphics, select the window that you want to save, go to File and select “Save Graphics.”

Select the format and resolution. I generally save them as TIFF Files at 8X screen resolution for presentation-quality graphics. I save at 16X screen resolution for publications. After you click Do It, you will be prompted to select the destination in which you want to save the graphics, similar to saving any other file.

4.4 Capturing Graph Preferences

Now that you have a graph that looks professional, you can save these preferences so that new graphs generated always have the same settings.

To do this, make sure the graph window is selected, go to the Graph tab and select “Capture graph prefs…”. Check all of the features you want to be saved (an example is shown below) and click “Capture Prefs.”
4.5 How to Make a Graph Macro

Graph macros are similar to capturing graph preferences but can be more specific (i.e. include axis labels for specific types of data), saving time if you have common types of data that you frequently work up. Here’s how to do it:

First, notice that there is a window of code in Igor that records all of your actions, shown here:
Copy the actions you want to have in your macro. NOTE: Actions applied to your specific traces ((Y_A) and (Y_B) in my case for this example) should not be copied, otherwise the macro will not work for data with different labels. Only copy things that can be applied generally.

Open a new procedure window by selecting Windows → Procedure Windows → Procedure Window.

On the second line of the procedure window, type the following, including spaces:

```
Proc name of procedure() : GraphStyle
```

For example, if I want my procedure to be named “General,” I would type the following:

```
Proc General() : GraphStyle
```

Then, starting in line 3, paste the actions you want in the procedure into the new procedure window. If you like all of the actions from this tutorial, the procedure window will look something like this:
Notice that things like setting the axis range were not copied since that is specific to the current data and is not generally applicable to all data. You can, however, make multiple graph macros to use for multiple types of data.

Save the procedure by clicking File → Save procedure copy…

When you download Igor, it should install a folder called “Igor Procedures.” I’d recommend saving the procedure in there as the desired name of the procedure.

Save your project and restart Igor.

To apply your macro in the future, make a graph (following this guide up to step 3b) and with the graph window selected go to Windows → Graph Macros → Your Procedure and all of your settings should be applied to that graph.
5 Adobe Illustrator

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5.1 Homework and In-Class Assignments

Before Class (due at the start of the workshop):

- Download Microsoft PowerPoint (see Microsoft Office primer)
- Make and save a theme using PowerPoint Master Slide (see Microsoft Office primer)
- Download Adobe Illustrator and start a new file (steps 1 and 2 in below primer)
- Save this file under a name and location you can easily find and open in class
- Using any combination of the PowerPoint and Illustrator tools described in these primers, start creating a scientific figure related to your current rotation project. If you do not know your rotation project yet, create a figure related to an undergraduate research project or laboratory assignment.

In Class:

- Come with any questions or confusion you have and we will work through them
- Continue working on your figure
- Discuss how to improve the following figure using use both PowerPoint and Illustrator:

![Diagram of a fuel cell]

Homework (due at the start of the following week):

- Finish your figure
- Export it as a high resolution (300 ppi) jpeg (if made in Adobe Illustrator)
- Import this into a PowerPoint slide
  - Apply the theme that you made for homework
  - Size figure appropriately for a presentation
- Turn in PowerPoint slide with the file name format
  LastName_FirstName_Figures.pptx
5.2 Why Use Adobe Illustrator for Scientific Figures?

For designing any image, a user must first decide which graphic format to use. The two common choices are Raster graphics and Vector graphics. Raster graphics are bitmaps, which is to say the image is a grid of individual pixels. The pixels have locations (x and y coordinates) but do not have any specific relationship to each other. Vector graphic are algorithmic, which is to say the lines/shapes/text are based on mathematical formulas. Lines/shapes/images do not have fixed locations but are rendered from calculation and are related to other objects mathematically. Compared to Raster, Vector graphics are easier to manipulate, can be scaled indefinitely, and will match the output resolution of any device. Vector graphics are generally smaller in size due to the luxury of not memorizing every single pixel. For most scientific figures Vector graphic design is the better choice; figures created in this format will materialize quicker, be easier to edit, and will be aesthetically appealing in more situations.

The difference becomes clear when zooming in on an inserted Raster vs Vector graphic in a document. The two figures below are the same Illustrator file. Image A was inserted as a Vector image (svg) while Image B was inserted as a Raster (jpeg). The difference is not visible zoomed out, but close up it becomes obvious.
A Brief Note on Graphic Design

This document is a small primer on the basics of graphic tools in Adobe Illustrator. These are the simplest tools, in the author’s eyes, that constitute a good foundation for new users. This document doesn’t say anything about the process of making graphics or really how to design a graphic. Those things could realistically be another 20 pages or more apiece.

A word of advice from an old teacher, a man who makes beautiful graphics. His advice is “always answer the why question. Answer it about every single detail of the graphic.”

Example:

- **Why** did you put a line on the document? It represents the ligand of a nanoparticle.
- **Why** is the line stroke 4 points? It is supposed to be ~4x as large as the other ligands which have strokes of 1 point.
- **Why** is the line 30 points long? Because the nanoparticle is 30 points wide and so they are symmetric in some sense.
- **Why** is the line where it is? Because it’s part of an array of 6 other lines each spaced 60° around the nanoparticle. It’s in this position to maintain symmetry which looks aesthetically pleasing. Also, the entire image is horizontal and vertical centered to improve symmetry.
- **Why** is the line that shade of blue? The ligand absorbs red light, also that shade of blue complements the nanoparticle’s shade of red and the 2nd ligand’s shade of green.

Answering these types of questions will improve your end graphic immensely and inevitably lead to discovering more powerful design tools.
5.4 How to download Adobe Illustrator

The Adobe Creative Cloud suite is available to all faculty, staff, and department student employees. This primer focuses on Adobe Illustrator, but all Adobe Creative Cloud applications (Photoshop, Acrobat, InDesign, etc.) are available to you.

To download Adobe Illustrator:

1. Visit this CASIT link: https://casit.uoregon.edu/faq/overview-of-adobe-creative-cloud-application
2. Scroll to “Installing the Adobe Creative Cloud desktop application” and click the link to “Adobe Creative Cloud desktop application page”
3. Follow the site step-by-step instructions to log in with your UO ID

5.5 Basic Document Setup

Initial Setup

Creating a new document in Adobe Illustrator is accomplished using Clt+N or by going to the File menu and clicking New Document. Since Illustrator is a Vector graphic program, document sizing need not be a primary concern at this point. However, if the user is interested in quantitative graphic design, I highly recommend using Points as the preferred Units (image 1). The preferred Units can be changed at any point during the graphic design, but Points will facilitate more precise relationships between objects.
Editing the document preferred Units can be accomplished by the shortcut Ctrl+K or by navigating the Edit menu to Preferences and General… (image 2). Once at the Preferences dialogue box navigate to the Units tab change the preferred Units (image 3).
Resizing after Document Setup

The composition space in Adobe Illustrator is known as an Artboard. Artboards can be added or edited after document setup by using the shortcut Clt+Alt+P or by navigating the File menu to Document Setup…. On the Document Setup dialogue box click Edit Artboards to access the editor (image 4).


The Edit Artboard button returns the user to the composition space and generates a transform box around the initial Artboard (image 5). Additional Artboards can be generated by clicking the paper button (blue arrow) or deleted by clicking the trash can (red arrow). Artboards can also be named by clicking the desired Artboard and then typing a name into the text box (green arrow). Pressing the escape key will close the editor and save your changes.
5.6 Handy Adobe Illustrator Shortcuts and Tricks

Learning a few Illustrator shortcuts can greatly increase work output and decrease user frustration. Since they apply to almost every situation, this section will cover the primary shortcuts used for selection and workspace navigation. **Brief summary:** press V to select entire objects, press A to select portions of objects, press Ctrl+Shift+A to deselect everything, press Alt and use the scroll wheel to zoom out/in, and press spacebar to reposition the stage.

Selection Key Presses (V, A, and Ctrl+Shift+A)

To generally select objects in Illustrator the *Selection Tool* can be used. This is the solid black arrow on the upper side of the tools toolbar. Clicking with this tool will select entire objects, grouped objects, and any related properties (e.g. fill color). By contrast, the *Direct Selection Tool* will only select the *Path* or *Anchor Point* that is being clicked on. Consider the square in image 6, if the upper right corner is selected with the *Selection Tool* the entire shape is selected. If the upper right corner is selected with the *Direct Selection Tool* only the upper right *Anchor Point* is selected.

*Image 5. The Artboard editor.*
The **Selection Tool** can be activated by pressing V on the keyboard, whereas **Direct Selection Tool** can be activated by pressing A. Alternatively, with one tool already selected, the other can be activated by pressing down the Ctrl key (Command for Mac). Generally speaking, selected objects/lines/points can be deselected by clicking an empty region of the **Artboard**. If the **Artboard** is sufficiently cluttered deselection can also be achieved using the keyboard shortcut Ctrl+Shift+A.

**Workspace Navigation Key Presses (Space and Alt+Scroll)**

It is likely, given use of other image manipulation programs, that you'll initially default to the magnifying tool and scroll bars for workspace navigation. These solutions work, however there are two ways to significantly expedite workspace navigation. First, holding down spacebar will transform the cursor into a hand; clicking and dragging with the hand repositions your view of the **Artboard** (note: this does not change any **Artboard** coordinates). Second, holding down the Alt key and then scrolling the mouse scroll wheel will zoom in and out on your workspace. Note: For users without scroll wheels, holding the Alt key converts the magnifying glass “zoom in” mode to “zoom out” mode.

### 5.7 Layer Control

For a mildly complex scientific figure (e.g. a band bending diagram) it is not uncommon for the final Illustrator document (.ai file) to include 100+ objects (e.g. paths, shapes, text, lines). The question becomes, how does the user effectively organize this information in a way that facilitates the presentation and future editing needs? The answer is **Layers**.

**Layers** are work organization constructs which can contain objects in Adobe Illustrator. Consider that Adobe Illustrator is similar in some ways to a physical sketchbook. For the analogy to be apt this must be a sketchbook in which the front cover and each page is transparent. We could say that each page of the sketchbook is a **Layer**. If you draw a circle on the first page (first **Layer**) and close the book you will see a circle through the transparent front cover. If you draw a square on
a page below (a lower Layer) then you will see the square unless the circle happens to be covering it up. Finally, each page of the sketchbook has a little tab sticking out where you can name/describe what that Layer contains. This tab enables you to quickly find/edit a select part of the overall graphic.

Layers allow the user to logically organize the separate pieces of the graphic. Layers also control which objects appear above/below others and can be used to hide pieces of the graphic which are not actively being worked on. By default, the Layers window (image 7) will be in the lower right-hand corner of the screen; if missing it can be activated by pressing F7 or by navigating the File menu to Layers. New Layers can be added by clicking the new page icon (blue arrow). Layers can be renamed by double clicking on the name (red arrow). An object is added to a Layer by first selecting the Layer and then drawing the object on an Artboard. If multiple objects are drawn on the same Layer a Sub-Layer will be generated for each one. Sub-Layers can be effectively used to group and organize similar objects. New Sub-Layers can be manually created by clicking the new page + arrow icon (green arrow).

In the example below multiple squares and circles are organized first by Layer and then by Sub-Layer. Since the squares are on a lower Layer, the circles will cover them whenever overlap occurs.

![Image 7. Example Layer window with squares and circles organized.](image)

Notice that the small blue circle is also partially obscured by the large blue circle. This is due to the large blue circle existing on a higher Sub-Layer.

Image 8 depicts a few additional useful aspects of layering. Clicking the eye next to any Layer will hide all of the Sub-Layers, whereas clicking the eye next to a Sub-Layer will only hide that Sub-Layer (blue arrow). Clicking the empty space directly to the right of the eye will lock the relevant Layer and thereby prevent edits of that Layer (red arrow). When an object is selected a shaded square will appear on the far right of the Layers menu denoting which Layer and Sub-Layer that
object is on (green arrow). The object can be moved to a new Layer by dragging the shaded square to an open square.

A well designed and maintained Layers window should be viewed as the foundation for any involved graphic design project. It's readily apparent that Layers allow the user to quickly find and edit select content. But use of Layers has more subtle advantages in that it allows the user to edit select content while not disturbing nearby/overlapping content. Also, a well-organized Layers window will facilitate other users who might edit the graphic and will allow the primary user to resume editing seamlessly after an extended absence.

5.8 Using the shape tool

The shape tool is the 9th icon in the tools toolbar and defaults to the appearance of a square with solid fill. By right clicking on the icon a list of various shapes can be accessed (rectangle, rounded rectangle, ellipse, polygon, star, and flare). To adequately discuss shapes this section will be broken up into “during-creation” and “post-creation” processing.

During-Creation Shape Tool

To begin creating a shape the user should select their desired geometry from the shape menu. Once selected, clicking and dragging any location on the document will generate a ghost image of what the shape will look like. Dragging further will effectively expand the dimensions of the shape. Letting go of the click will finalize the shape on the document. But before letting go there are a number of options that allow manipulation of the shape. Different key presses produce various effects depending on which tool is being used:

- Holding the alt key during the click+drag process will re-center the shape around the initially clicked point.
• Holding the **shift key** will ensure that the *Rectangle Tool, Rounded Rectangle Tool, and Ellipse Tool* all generate perfectly symmetrical shapes (i.e. a square, a rounded square, and a circle).

• Holding the **shift key** while using the *Polygon Tool* and the *Star Tool* will simply orient the shape’s axis vertically on the *Artboard*.

• Holding the **ctrl key** while using the *Star Tool* allows the user to change the distance between the tip points and the inner points.

• Pressing the **up key** while using the *Polygon Tool* will increase the number of sides by 1.

• Pressing the **up key** while using the *Star Tool* will increase the number of points by 1.

• Pressing the **up key** while using the *Rounded Rectangle Tool* will increase the degree of rounding.

• Pressing the **down key** while using the *Polygon Tool* will decrease the number of sides by 1.

• Pressing the **down key** while using the *Star Tool* will decrease the number of points by 1.

• Pressing the **down key** while using the *Rounded Rectangle Tool* will decrease the degree of rounding.

**Post-creation Shape Tool**

After finalizing the shape the dimensions can be further manipulated by clicking the shape and dragging the *Anchor Points*. The *Control Bar* along the top of the screen can be used to further modify shape properties (image 9). The first box (blue arrow) is used to select the fill color of the shape. The second box (red arrow) is used to select the color of the outline. Both of these can be set to null (no fill / no stroke) if desired. The stroke panel (green arrows) allows the user to manipulate the stroke thickness, the width profile, and the brush definition. The transparency panel (yellow arrow) allows the user to set opacity of the shape.

![Image 9. First half of the Control bar.](image)

The *Control Bar* can also be used to precisely align the created shapes. The leftmost box in image 10 can be used to toggle the frame of reference (blue arrow) between the current selection, a key object, or the artboard. By clicking Align to Artboard the menu expands and allows horizontal alignment to the left/center/right and vertical alignment to the top/center/bottom (red arrows). The icon with 9 boxes allows the user to select which part of the object is used for alignment (green
arrows); the X and Y coordinates are the coordinates of the aligned object (yellow arrows). W and H are used to set the height and width of object while the lock depicted between them dictates whether or not those two dimensions scale with each other or individually (purple arrows).

Examples of different properties can be seen in image 11. The red star is set to no stroke and rotated slightly. The ctrl key was used during creation to create sharper points and the up key was used to increase the number of points. The teal rounded rectangle has a 50% transparency and slightly more rounded corners via use of the shift key. For the polygon the down key was used to eliminate one side and no fill is selected. Finally, all three shapes are aligned to the vertical center of their composite composition space.

Image 11. Example of various shapes created with the Shape Tool.
5.9 Making a 3D Shape

To make a 3D shape, you revolve a 2D shape around its center. For example, to make a sphere, start with a circle. Make sure it has an outline color. Using the Direct Selection Tool (white arrow), select and delete one anchor point to form a half-circle (Image 12).

![Image 12: Starting from a circle, select and delete the left point.]

Select the half-circle, then navigate to the Effect menu to the 3D option and select Revolve…. (Image 13) In the Revolve menu (Image 14), make sure the Preview box is checked (Red arrow). Moving the box changes the angle of rotation about the axis.

![Image 13: Navigate to the Revolve button]
You can make a variety of 3D shapes using this method (e.g. a cone by rotating a triangle or cylinder by rotating a rectangle). However, for unique shapes moving or rotating the 3D figure after creating it will change the axis of rotation and ruin the shape (Image 15).

To fix this, the 3D shape must be expanded. Select the shape, navigate to the Object menu and select Expand Appearance (Image 16). After doing so, the figure is isolated as a flat shape and can be moved.
**Image 16:** Object menu to Expand Appearance

**Image 17:** 3D figure rotated 90° after Expand Appearance
5.10 Using the Pen Tool

General Path Creation

The Pen Tool’s importance in creating scientific figures is difficult to overstate. Any shape or path that is not of some regular geometry (which would be created with the Shape Tool) can be produced via this tool. The Pen Tool also enables precise control over the curvature of paths. On the surface the Pen Tool is straightforward to use, clicking the icon (5th tool on the Tools Menu) and clicking anywhere on an Artboard begins a path. A second click will continue the path by drawing a line to the newly generated Anchor Point; a third click will do the same and this trend will continue until the pen tool is deselected, the path is completed back to the initial point, or the esc key is clicked. During the initial generation of a path two key presses can be of use:

Pressing the shift key can be used to generate paths at any multiple of a 45° angle.

Holding the left mouse click at each point can be used to create curvature in the initial path. Doing so will produce curvature handles which can be manipulated to change the extent of curvature (image 18).

![Image 18. Anchor points are created from left to right. The second and third point were produced while holding the shift key to generate 0° and 45° angles. The fourth point was generated while holding the left mouse click to produce the curvature handles.](image)

Closing the path, by clicking on the initial Anchor Point, will generate a shape which can be manipulated as per the geometric shapes previously covered. Right clicking the Pen Tool allows access to three other tools: Add Anchor Point Tool, Delete Anchor Point Tool, and Anchor Point Tool. The effects produced by these tools are displayed in image 19. The Add Anchor Point Tool can be used to add a new Anchor Point to a pre-existing path (blue arrow). The Delete Anchor Point Tool will remove an existing Anchor Point. The Anchor Point Tool will generate curvature handles (if they do not already exist) on an anchor point and allow the user to manipulate them (red arrow). Keep in mind that the Direct Selection Tool can be used to move a single Anchor Point to a new location (green arrow).
Image 19. Same as image 18 but with 1st anchor point moved down via the Direct Selection Tool, a new anchor pointed added after the 1st via the New Anchor Point Tool, and the Anchor Point Tool used on the previously 3rd anchor point to apply curvature.

Stroke Dialogue Box and Scissor Tool

Paths can be further edited by using the Stroke dialogue box which can be accessed by navigating the Window menu to the Stroke option or with the shortcut Ctrl+F10. Most notably, the Stroke dialogue box can be used to convert the path to a dashed line, to add arrowheads to the path ends, and to change the weight (image 20).

Image 20. The Stroke dialogue box.

Editing single anchor points is straightforward, as they can be individually selected with the Direct Selection Tool. However, editing path segments in this way is not possible. A feasible way to individually edit a path segment is to have initially made the path segment its own path (and then connected it to the larger path). This approach requires some foresight and is not useful after the path has already been created. Instead, a path can be split up by using the Scissors Tool. The
Scissors Tool can be found by right clicking the Eraser Tool in the tools toolbar or by using the keyboard shortcut C. Clicking the Scissors Tool on any part of the path will generate two overlapping Anchor Points (or just one if you clicked an already existent Anchor Point) and divide the path into two new paths on either side of the click. Image 21 demonstrates use of the Scissors Tool and the Stroke Dialogue panel.

![Image 21](accessing_the_scissors_tool_from_the_toolbar.png)

5.11 Using the Type Tool

The type tool is relatively straightforward to use for most foreseeable scientific tasks. It can be accessed from the tool bar (the 7th icon from the top) or with the keyboard shortcut T. Once selected, clicking a location on the Artboard will initiate a text box and the user can then input text. The control bar features many of the same options as for shapes but with the notable addition of the Character Panel (image 23). The character panel can be used to select the font (blue arrow), select the font style (red arrow), select the font size (green arrow), align the font (yellow arrow), and warp or distort the font (purple arrow). An example of text warp is depicted in image 24; there are many different warps available.

![Image 22](scissors_tool_used_to_break_the_path_into_two_segments_blue_arrow_the_stroke_dialogue_box_was_used_to_add_a_dashed_line_to_the_smaller_segment_red_arrow_the_stroke_dialogue_box_was_also_used_to_add_an_arrow_to_the_larger_line_segment_green_arrow.png)
Type Character Dialogue Box

As with strokes, there is a dialogue box for characters which gives the user finer control over the vector image. The Type Character dialogue box can be accessed with the keyboard shortcut Ctrl+T or by navigating the Window Menu to Type and then Character. Most notably, the Type Character dialogue box allows the user to add subscripts, superscripts, and underlines. Although it may be necessary to click the button in the upper right of the dialogue box to gain access to these options (image 25).

Eyedropper Tool (Text Use)

In many programs the Eyedropper Tool is used for sampling color palettes. While it maintains that functionality in Adobe Illustrator it can also be used to sample text. To do so, use the Selection Tool to select text that you wish to change. Next, select the Eyedropper Tool by using the shortcut Ctrl+I or simply by navigating to it in the tool bar (21st from the top). Upon activating the Eyedropper Tool the cursor will become an eyedropper. Finally, left click the text you wish to sample; the initially selected text will adopt all the properties of the sampled text.
5.12 Using the Clipping Mask Tool

On occasion you may run across situations where it would be advantageous to show a select part of some group of objects. One easy option is to remake the objects without the undesired content present. However, this approach can be tedious and sometimes detrimental (consider the case where you cut a complicated polygon into numerous pieces, delete the unwanted pieces, and then later realize you needed the whole polygon). A better approach is to use a Clipping Mask, which allows the user to show a select area while still keeping the group of objects intact. The Clipping Mask can be activated by using the keyboard shortcut Ctrl+F7 or by navigating the Object menu to Clipping Mask and selecting Make (image 26).

![Image 26. Navigating to the Clipping Mask Make button.](image)

To use the tool a group of objects should be selected which the user wishes to mask/clip. Additionally, one of the selected objects should be the intended Clipping Mask. Adobe interprets the object on the highest Layer or Sub-Layer as the Clipping Mask. Consider the example below wherein four rectangles will be masked by a circular Clipping Mask. The circle is placed partially overlapping the rectangles and on the highest layer (note: the fill or lack of fill is not important as clipping is based on the geometric area of the Clipping Mask). Upon pressing Ctrl+F7 the edges
of the rectangles which extend beyond the circle will be clipped from view. Also notice that the 
Layers Window changes to reflect the presence of the Clipping Mask (image 27).

![Image 27. Four rectangles before and after applying a clipping mask. In the Layers window the path gets renamed as “Clipping Mask” and a Clip Group is formed.](image)

After a Clipping Mask is formed, double clicking on any of the objects within it will allow the user to change the position of those objects (image 28). Clipping Masks can be released by selecting the Release option directly below Make in the Object menu.
5.13 Saving and inserting an image

Select the file format for your application
The most common vector formats used are Scalable Vector Graphics (SVG), Enhanced Metafiles (EMF), and Portable Document Format (PDF), and Adobe Illustrator (AI). Any vector-based file can be opened and edited in Adobe Illustrator.

The type of format to save your image depends on your application. Raster images are best for screen applications, such as Power Point presentations, while Vector images are best for inserting into professional PDF documents, for example fellowship applications. Some academic journals accept PDF or AI files directly, but most only accept Raster images require a high resolution JPEG.

Saving a file
To export a figure, navigate to Export under the File menu (Image 29) and select the file format (Red arrow).
When exporting as a vector image, there are advantages and disadvantages to each format, and some are better than others depending on operating system (Mac vs PC). Below are a few tricks for saving as a vector image. If the exported image is not correct when inserting into a document, troubleshoot with the following tricks:

- If saving as svg, convert to outlines (Image 30)
- Check that all 3D shapes are expanded (see instructions for making a 3D shape)
- Convert text to outlines (Image 31). Select all text, navigate to the *Type* menu and select *Create Outlines*
- Make sure the original .ai file is larger than the size you want in your word doc
- Expand again (Image 32)
5.14 Additional useful information

Guides and Alignment

A major advantage to Adobe Illustrator is the capacity to create objects that are quantitatively related to each other. This is enabled by the Vector format and the various guides build into the program. In this section we'll look at the default Smart Guides, User Created Guides, and Grid alignment.

Smart Guides

Smart Guides are enabled by default in Adobe Illustrator and will offer helpful suggestions when manipulating objects (shapes/paths/text). For instance, when moving a square in the vicinity of a second square the smart guides will show when their midpoints align, when their edges align and when one square’s midpoint aligns with the other square’s edges. Smart Guide functionality can be modified by navigating the Edit menu to Preferences and then Smart Guides… (image 33). It can be useful to lower the Snapping Tolerance when working with very detailed sets of objects.
User Created Guides

Users can create Guides in the document that facilitate alignment. Objects will snap to these lines when brought within the Snapping Tolerance. To create a guide the user must first turn on the ruler by using the keyboard shortcut Ctrl+R or by navigating the View menu to Rulers and Show Ruler (image 34). Once the rulers are active they will appear along the top and left sides of the screen (blue arrows). To create a guide the user must click and press on either ruler and drag into the center of the Artboard. Doing so will generate a thin teal line which can be positioned freely within the composition space (red arrows). Guides can be deleted, hidden, or locked by navigating the View menu to Guides (green arrow).
Grid Alignment

It is also possible to align objects to preset grid lines in Adobe Illustrators. These can be activated by navigating the View menu to Show Grid or by using the keyboard shortcut Ctrl+” (purple arrow in image 34). The Grid can be edited by navigating the Edit menu to My Preferences and Guides & Grid… (image 25).

As can be seen in image 36, the Guides and Grid tab of the Preferences dialogue box allows the user to control the spacing between major gridlines (blue arrow) and minor gridlines (red arrow).
Image 36. Guides and Grid tab of the Preferences dialogue box.
6 CrystalMaker

Point person: Tawney Knecht (tknecht@uoregon.edu)

6.1 Download Information

- Go to https://researchguides.uoregon.edu/chemistry/software for general instructions
- Click on link “Download from CrystalMaker”
- Download CrystalMaker, CrystalDiffract, and SingleCrystal from the CrystalMaker website.
- Obtain site license information from the Science Library. Contact: Annie Zeidman-Karpinski, annie@uoregon.edu

6.2 Online Tutorials

This primer will go through how to open .cif files, view and manipulate crystal structures in CrystalMaker. More comprehensive CrystalMaker tutorials are online on the CrystalMaker website. Please consult these to gain more familiarity with this crystallography software.

Tutorials are found here: http://crystalmaker.com/crystalmaker/video-tutorials/index.html

6.3 Opening a Structure

The Structures Library

When you download CrystalMaker, you will get access to a library of structures. From this library, you can access basic structure types and then edit the structures to include the desired atoms. Browse through your library to see what structures are available.

ICSD

More often than not, the crystal structure you need already exists in the Inorganic Crystal Structure Database (ICSD). Go to the ICSD website (https://icsd.products.fiz-karlsruhe.de/) and click on “LOGIN to ICSD” in the top right corner of the screen. This should bring you to this page:
Enter the desired atoms in your structure in the “Chemistry Composition” line (separate elements by spaces), and restrict the number of elements in the following “Number of Elements” line. In the example above, the structure for CeO$_2$ is being searched for, so “Ce O” was entered in the chemistry composition line, and the number of elements was restricted to 2.

Click “Run Query,” and this will generate a search.

Check the box next to the desired structure and then click “Show Detailed View.” If this structure is indeed the structure you want to open, click “Export Cif” in the top right corner. This will download the .cif file, which can be opened in CrystalMaker.

6.4 Viewing Crystals

- To rotate the crystal, simply click to “grab” the crystal and move your cursor around.
- Hold SHIFT and click and graph the crystal to only rotate in the axis perpendicular to your screen
• You can also rotate using the icon in the toolbar.
• View your crystal along a certain direction by clicking the orient icon and typing in the facet you want to view. In the below example, the 110 facet was entered as the View Direction

• Change the model by clicking on the “Model” in the top toolbar. Here you can select a number of model options.

• Change the size of your structure by clicking the Range icon. Here, you can:
  o Expand or Contract range: this expands/contracts the structure equally in all directions
  o Enter specific axial range limits along various axes

• Turn your structure into a cluster or nanocrystal by clicking on Cluster.
  o Enter in your central atom
  o Enter in the desired radius
  o Click “Reset Cluster Size”
6.5 Changing Atom Colors, Radii, and Bonds

- To bring up the necessary menu, click on Inspector in the top right corner of the screen. The following menu should appear, if not already visible:

  ![Inspector Menu]

- Click through these to see what they can do.
- To change atom color and radii, click on the second icon with the sphere and pyramid.
  - Edit the radius (if ever necessary) in the column “r[Å]”
  - Edit the color in the column “Col”
  - Edit the atom style in the column “Style and Label”
  - And so on…

![Atom Style and Color]

- To change bond type, click on the icon
  - Click on the 3D image of the bond to edit the bond type and appearance
  - And so on…
6.6 Exporting Images

To export graphics, go to File ➔ Export Graphics ➔ 2D Graphics

Select the desired settings and save as prompted.
7 Additional Resources

Please refer to the University of Oregon Science Library Research Guides website for more information on several useful databases and software:
https://researchguides.uoregon.edu/chemistry

7.1 Software
- Avogadro
- Crystallography
  - Mercury
  - GSAS
- Dropbox
- Figures
  - GIMP
  - Inkscape
- Graphing
  - Origin Pro
  - MagicPlot
- ImageJ
- Reference managers (specific ones may be preferred by some labs)
  - Endnote
  - Mendeley
  - Zotero

7.2 Databases and Online Resources
- Cambridge Structural Database (CSD):
  https://www.ccdc.cam.ac.uk/structures
- ChemSpider:
  http://www.chemspider.com/
- Inorganic Crystal Structure Database (ICSD):
  https://icsd.products.fiz-karlsruhe.de/
- NIST Chemistry Webbook:
  https://webbook.nist.gov/chemistry/
- Scifinder:
  https://scifinder.cas.org/
- Spectral Database for Organic Compounds (SDBS):
  https://sdfs.db.aist.go.jp/sdfs/cgi-bin/direct_frame_top.cgi
- Web of Science:
  https://apps.webofknowledge.com/
8 Shannon Boettcher Lab Guide

1. I like students to use Endnote for references. They often use a mishmash of other software that can’t get all the formatting correct. Endnote is not ideal in many ways, but it does the formatting right and is what most folks use.
   a. I have a journal abbreviation library that can be imported and takes care of all the journal abbreviations.
   b. Sentence case for reference titles unless otherwise noted by Journal style

2. Since we have illustrator as a standard software all students should just learn how to use it. Photoshop is not really that important since we don’t manipulate photos when we publish SEM etc.

3. Graphing – we use Origin. It requires an expensive license but is very user friendly, so students will get access instructions during their rotation.

4. For plotting etc.
   a. no serif fonts
   b. font sizes commensurate with other in the journal article (i.e. 6 pt or larger)
   c. close in borders around graphs
   d. don’t use legends unless absolutely necessary, label data directly on plot instead
   e. take into account colors for contrast and for color blind folks
   f. graphs should be readable when printed in black and white
   g. effective use of white space with insets, illustrations etc.

5. Graphics
   a. No excessive use of 3D shapes just for the sake of it
   b. Use simple clean line art for most cases
9 Carl Brozek Lab Guide

General Expectations:

- You are expected to help maintain a good safety culture by adhering to requirements and reminding others about requirements when necessary.
- During the COVID-19 pandemic, you are expected to show up for your scheduled shifts. If you will not be in the lab for the majority of your shift, the shift should be marked available with as much advance notice as possible.
- When the pandemic subsides, you are expected to be in the lab or office during normal working hours if you do not have class or teaching responsibilities.
- Do not work in the lab alone.
- You are expected to ask questions! Don’t stay silent about things you don’t understand. Anyone in the lab will be happy to help you. (Ask your direct mentor first though.)

Software Needed:

- General: Microsoft Office
- Graphing and Figure Making: Igor Pro, ChemDraw, Vesta, Adobe Illustrator
- Data Interpretation: MestreNova, EVA
- Crystallography: CrystalMaker/CrystalDiffract, Mercury, GSAS
- Reference Manager: Zotero/Mendeley
- Also have: A Scifinder account, a RSS Feed Reader (Newsblur, Feedly, Old Reader)

Figures:

Igor:

- **Axis Options**: No axis standoff, mirror axis (no ticks)
- **Auto/Man Ticks**: Check minor ticks
- **Ticks and Grids**: Major Length 3.5
- **In Graph options**: Width: Absolute 3.5, Length: Aspect 0.62
- **In Modify Trace Appearance**: change trace color from bright red. If you are graphing data at particular points, rather than a continuous trace, choose “line with markers” and use circular markers.
- **To label traces**: Use “Annotate Graph” and drag your labels close to the data. Do not use legend. When there are multiple labels, align them nicely.
- **When you have these general settings** (No axis labels yet), go to Graph/Capture Graph Pref… to save these preferences for all eternity.

Adobe Illustrator:

- Figures should follow the standard group guidelines: 3.25-in wide panels with 0.62 aspect ratios, 9-pt Arial font throughout, 0.5 pt line thickness, minimize dead white space, and ask yourself “does my figure clearly convey the message?”
- Start by making your artboard the appropriate size for the figure you are making i.e. single or double column.
• Color choice should be unsaturated, color-blind friendly, and HTML-friendly. Use consistent color schemes.

**PXRD:** Y Axis: Intensity (a.u.) No ticks or numerical labels necessary. X Axis: $2\theta$ Symbol ‘$\theta$’ in ‘Characters’. Stacked your patterns, do not overlay them. Two methods to accomplish this:

a) When New Graph, choose to put all y waves on a different y axis. Then, in Axis Options, use “between % and %” to move the traces up and down. Don’t leave axis gaps.

b) Put all patterns on the same y axis in New Graph. Then, in Modify Trace Appearance, check “offset” and use the y axis offset to move the traces up and down. You can additionally use y% to increase or decrease relative intensity.

Plot against a simulated or expected powder pattern. Label with Miller indices if appropriate.

**IR:** Overlay normalized IR spectra. Label with the appropriate names for each trace. Annotate traces with the important bands of the material. Overlay traces with target material, starting materials, or other related compounds.

**UV-Vis:** Overlay normalized UV-Vis spectra after correcting for lamp shifts. Label with the appropriate names for each trace. Annotate traces with the important transitions. If looking at a transition metal-complex conduct ligand field analysis as necessary. For diffuse reflectance data, use the Kubelka-Munk function to transform the reflectance into absorption. The Y axis should then read “Normalized F(R) (a.u.)”. For general UV-Vis x-axis is in wavenumbers with increasing energy towards the left. Tauc plots use eV as the x-axis.

**Chem Draw:** Use to draw reaction schemes. General settings: ACS Document 1996, line thickness 0.0118 in. Include reaction conditions, all relevant counterions, and side products. The reaction should be balanced.

**VESTA:** Use VESTA style file. Make sure you can see the structure clearly. A good way to do this is look at the structure from a, b, or c, then use the arrow keys to rotate it off-axis in one direction. Use the “Boundary” function to play with how much the material is visible. You should see enough of the structure to see the topology clearly, while also still be able to see detail. **Delete all dangling bonds.**

**CrystalMaker/CrystalDiffract:** Use CrystalMaker/CrystalDiffract to view crystal structures of materials that you have a .cif file for, or to simulate powder patterns. Open your .cif file in CrystalMaker and go to Calculate > Powder Diffraction > New Pattern. This will open CrystalDiffract. From here, note the indexed peaks and File > Export Diffraction > Profile. Load in Igor as a .txt file.

**Presentations:**

• Use an Assertion/Evidence style talk to make your story clear. Titles are assertions: the key conclusion of the slide. Evidence is the figures and minimal text on the body of the slide.
• When presenting characterization data for a product, the chemdraw scheme for the reaction by which the product was made should be at the top of the slide.
• Include relevant citations in ACS style at the bottom of the slides. Include all authors; do not use “et al.”

**Monday Morning Meeting:**
• Have at least one fully updated E-notebook page to share in MMM
• Title pages with physical notebook code (Ex. CK1-001) and a short description
• Include a balanced reaction scheme from ChemDraw
• Include a reaction table and a procedure
• Include at least one worked-up figure of data you collected
• Be prepared to discuss data interpretation / conclusions, and your plans for the upcoming week

Lab Notebooks and Record Keeping:

The purpose of the physical notebook is to be a complete record of everything you do in lab.

Every experiment should include:

• A descriptive title
• A purpose
• A reaction scheme
• A table of the reagents used (Molecular weight, Amount, Moles, Equivalence, etc)
• A detailed procedure
• Characterization section indicating what measurements were done, on what instrument, and the file name and location.
• Conclusions (Yield, Success/Failure, etc)

Use of the enotebook:

• Every experiment should include the same sections as the physical notebook. It is advantageous to write out formal procedures for future use.
• Reference relevant papers.
• Upload images from Chemdraw for your reaction schemes.
• Upload photos and pictures of data collected and add them into the e-notebook pages. Caption all items clearly and descriptively.
• Update your experiment status accordingly. IE don’t leave all your experiments as “In Progress.”

When attaching data to show in the enotebook scroll down the page to the Attach a file box > click then upload the appropriate file as either a .jpeg or .png.> then scroll to Attached files and click insert at cursor position > resize image as appropriate.
The primary pieces of software that we use are ChemDraw and MestreNova. Below are examples of reaction schemes and NMR analysis that are presentation-ready. Also included are specific expectations for PowerPoint presentations (including information on graphing data).

**Rules for PowerPoint Presentations**

- Sans serif font (hard to tell the difference between c and e, e.g., in serif fonts)
- No points smaller than 14 (12 ok for references and graph axes)
  - Point 18
  - Point 16
  - Point 14
  - Point 12
  - Point 10
  - Point 8
- Use animations to help guide the audience’s attention
- No superscripted o’s or 0’s → use a degree sign!

![Example of reaction scheme and NMR analysis](image)

Increased the size of the superscripted text so it’s easier to read!

**Degree sign shortcut**

Windows: Alt+0176
Mac: opt+shift+8

**En dash shortcut**

Windows: ctrl+minus key (the one on the number pad) or alt+0150
Mac: opt+minus key

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**How to Present NMR Data (and spectra in general)**

- All structures are the same size (and same size as previous slide)
- Bonds are thick enough to see and print well
- Reaction cleanup tool was used (ctrl+shift+X)
- No weird bond lengths (use molecule cleanup tool (ctrl+shift+K) if necessary)
- Properly labelled with the structure
- Solvents and impurities labelled
- Important area emphasized
- Fonts are ≥12 pt

![NMR spectra example](image)
11 Mike Haley Lab Guide

Data Plotting:
- Font: Arial
- Font sizes should be legible from arms-length away for most figures, generally 10pt at minimum
- Make Excel fonts black, and borders black and bold enough
  - Depending on figure, major tick marks on axes should face out and minor tick marks do not have to be included
- Make lines/curves in most plotting programs 1.5pt or 2pt to help them stand out

Figure Making/Presentations (and how to give a talk):
- Powerpoint preferred (though not mandatory)
- All ChemDraw structures must be the same size
  - Copy/paste then expand all by the same percent (typically ca. 120-150% size)
  - Also make sure to paste all as images or all as ChemDraw embedded files, not a mix
- Slide titles should be a short description of the key point a slide is trying to make
- All slides should have at least one figure
  - Animations, boxes, and arrows can help break down bigger figures or tables and guide the audience as well as the speaker.
  - Do not go overboard with the animation (max 3-4 per slide)
- Keep words to a minimum
  - Bolding key words in longer sentences can help if long statements need to be added (i.e., quotes, long definitions, etc.)
- References at bottom of each relevant slide, use consistent style and consistent font size
- Use simple slide styles - wouldn’t hurt to make your own template to use throughout grad school. No dark backgrounds as it makes lettering hard to read

Routine Software (most are available at https://software.uoregon.edu/ with a UO account):
- ChemDraw (structure drawing)
  - ACS Document 1996 style template
- SciFinder - not software, but not everyone knows how to use it
- MestreNova (NMR processing)
  - Make fonts big enough (change from default)
  - Delete the background grid
  - Change x-axis label to “chemical shift (ppm)”
- File transfer program
- VPN
- MS Office 365
- Other possible software
  - Avogadro
  - Mercury (x-ray structures)
  - Vesta
  - Zotero/Mendeley (literature managing software)
  - Talapas account (UO supercomputer)
- Chemistry reference resolver is a very helpful tool!
**Standard Skills:**
- Make subgroups in ChemDraw (watch out for copy and paste errors)
  - Yields on all reactions
  - ChemDraw in ACS format
  - Have NMRs of all reactions ready to show
  - Also have starting material NMRs ready for comparison
- Lab notebook/record keeping
  - Draw reactions
  - Have quantities table
  - Write out procedure and yields, you want to write down enough to be able to look back and repeat it easily
- If making a new compound be mindful of characterization
  - Always obtain clean 1H, 13C NMR spectra
  - Save some of the clean sample for MS
  - Other NMR if applicable (e.g., 31P), and other characterization (e.g., UV-Vis, fluorescence) of final compound
- Get NMR training from Nanette (can register for training online)
  - Especially with Icon NMR

**Graduate School and Professional Skills Beyond Research:**
- How to make a CV
  - Best way to learn is to look at examples from bosses and mimic their style
  - Each CV tells a story. Organize the sections based on relevance (i.e., education history, then research experience, then professional experience, then extracurricular experience, and so on)
- How to write a manuscript
  - First and foremost, know that it isn't something that is quick and easy
  - Go onto the website of the journal that you are going to submit to and check early and often for formatting/length requirements
  - Outlining a manuscript is a great way to figure out what figures you may need, as well as what references you may need for key points each section wants to make
  - Emulating previously published papers from the lab (but not plagiarizing) is a good start
  - Start on the supporting information document early so you can make sure you have all the characterization you need to submit. If you do this too late, then you will have to wait on benchwork to submit instead of finishing it off while writing
  - Ask your peers (in your lab or not) to help develop ideas and edit drafts. The more refined of a draft you give to your PI, the better it will turn out in the end

**General Expectations:**
- When not teaching/in class most school day hours we expect to see you in lab
  - Could be grading or studying, but do it at your desk in lab (though likely this can happen only when the covid pandemic subsides)
- Mistakes are OK since they are a part of learning anything
  - Ask those around you how to avoid the mistake and build your knowledge from that experience
- In our lab, people are expected to be receptive and respectful to other people’s opinions and such
  - We strive to cultivate a positive lab environment and reach compromises on any decisions that may have driven a wedge between people in lab
- If something makes you feel uncomfortable, whether it be a reaction or something said, please let us know and we will work through it and resolve it however is best.
  - A good rule of thumb is that if you are not sure about the safety of something, then ask someone else first.
    - Though we have a formal “safety officer”, everyone in lab is more than capable of answering these questions and/or giving the required trainings.
    - Do not work in lab alone.

- General schedule:
  - Subgroup happens once per week, runs ~1 h.
  - Group meetings happen once per week (often Wednesday night), run ~2 h.
12 Ramesh Jasti Lab Resources

Making Figures

Fluffy style

1. Create .pdb file in avogadro
2. Open in QuteMol and save as a .png
3. Open in photoshop and color
   a. Use the "Quick Selection Tool" to select what will be a certain colour
   b. Color by adding a Hue/Saturation layer and selecting colorize

Rotating GIFs

1. Open in QuteMol
2. Save as rotating .gif, use between 100 and 200 as spin speed

Alternative

1. Open as a .pdb file in Mercury
2. Click animate and begin the molecule spinning
3. Use Screen to GIF to record the molecule spinning

Opaque molecules

1. Copy ChemDraw into PowerPoint
2. Use the freeform drawing tool to outline the front shapes that will be opaque
3. Copy these shapes back into ChemDraw and fit them into place
4. Send the shapes to back and then send all bonds that should be blocked by the front shapes to back
5. Go back to PowerPoint and draw the back shapes
6. Copy them into ChemDraw, fit them into place and send to back

Nanotubes

1. Open Avogadro and find the "Nanotube Builder" tool
2. Insert the desired chiral vectors and select the desired length (15 Å is good for tubes, 3 Å makes a CPP)

3. Do not minimize, save as a .mol file

4. Open in ChemDraw and orient to preferred perspective using the Structure Perspective tool

5. Flatten the molecule and ensure all front bonds are in the front and back bonds are in the back

6. Bold all front bonds

**Orbitals**

1. Open ChemDraw file in Spartan

2. Minimize the structure

3. Do a calculation from Setup>>Calculations (Energy at Ground state with Semi-Empirical AM1 from Current geometry is quickest)

4. Go to Setup>>Surfaces and click Add. From here pick the surface you want and set the resolution to as high as possible

5. Go to Model>>Line

6. Then deselect hydrogens in the same menu

**Large molecules**
1. Draw the molecule using ChemDraw (for fullerenes, see Schlegel diagrams) and save a .mol file
2. Open in Avogadro, minimize using the MMFF94 forcefield, and save as a .mol file
3. Open in ChemDraw and orient to preferred perspective using the Structure Perspective tool
4. Flatten the molecule and ensure all front bonds are in the front and back bonds are in the back
5. Bold all front bonds

Things on surfaces

1. Open surface crystal structure in Mercury and extend the crystal plane in the appropriate directions (Calculate>>packing/slicing) to form a surface
2. Save as a .pdb
3. Do same with object to be placed on surface
4. Open both in avogadro and copy one structure into the other and position
13 Darren Johnson Lab Guide

Software to have downloaded (and is free)

- Microsoft Word
- Microsoft PowerPoint
  - For subgroup and group meeting presentations
- Microsoft Excel
  - For data analysis
- Microsoft OneNote
  - For our online notebooks
- ChemDraw
  - For drawing all chemical structures
- Mestrenova
  - For NMR analysis
- Avogadro
  - For simple chemical structure optimization
- Adobe Illustrator
  - For figure creation
- Matlab
  - For data analysis
- CiscoConnect
  - To access the VPN when you are off-campus
- WinSCP
  - To access NMR files
- Dropbox
  - Free through the University. Generally good to have things backed up.

Group Meetings (~1.5 hours, once per week)

Our group meetings are divided into 4 sections:

- Good news
  - People are encouraged to share their good news from the week, whether it is lab-related or not
- Lab business and safety
  - Anyone can bring up a lab business or safety concern
- Equity and Inclusion
  - Topics of equity and inclusion are discussed every week, whether it is lab-related or not
- Scientific talk
  - Length varies for purpose of talk. Rotation students will be expected to give two 15-minute presentations throughout the term. The first presentation will be at the beginning of the rotation, outlining the project motivation and expected research plan. The second presentation will be at the end of the term and serve as a practice rotation talk.
At the beginning of our group meeting presentations we include a brief ‘life update’ in which we can talk about updates in our lives, or introduce ourselves if we’re new.

**Subgroup (~1 hour, once per week)**

For subgroup we meet in smaller groups with the other researchers on our project. We talk about what we’ve done the previous week, problems that have occurred, and plans for the next week. Subgroup is to ask questions and get help on places that you’re stuck. Subgroup is also to keep the group informed of your research progress. Come prepared with your data in a way that is easy to talk through. For example, you could make an informal PowerPoint with a synthetic scheme showing a reaction that you just ran and the NMR of the reaction mixture.
Typical DCJ lab projects involve synthesizing a thin film, following its evolution as a function of annealing temperature, and measuring the electrical properties of the material. One of the most common figures we make is of stacked x-ray diffraction patterns graphed as a function of annealing temperature (Figure 1). The patterns are stacked so that the lowest temperature annealed sample (the as-deposited) is at the lowest intensity and the highest temperature annealed sample is at the highest intensity to enable a clear comparison of changes with increasing temperature. From a stylistic perspective, we prefer the patterns to be the same color (black) when comparing the same sample at various temperatures. If comparing several different samples at the same temperature, then different colors may be used to add clarity to the discussion. The line width (1.5) should be consistent for each pattern. The patterns should be spaced so that the reflections in different patterns do not overlap and there is space to indicate the annealing temperature or sample identification, usually on the right side if the pattern allows for it. The font should be Arial with the axis titles and temperatures as 14-point font and the x-axis, Miller indices, and legend at the top as 12-point font. The Miller indices are indicated via normal, bold, or italic fonts for different phases. It should be noted that the intensity is arbitrary so there are no numbers or tick marks on the y-axis for these graphs. Units are indicated after the axis description with a “/”.

Figure 2: Examples of other common DCJ lab figures: amounts of material (a), composition of binary samples (b), and resistivity as a function of temperature (c).

For a presentation especially, figures are better tools than tables to illustrate data. Examples include amounts of material as a function of annealing temperature, composition as a function of film thickness or annealing temperature, and electrical properties such as resistivity and Hall effect. The same font guidelines apply to these figures. Additionally, markers should be 7.0 in size. In Figure 2a, the amounts of material in a single precursor are followed as the sample is annealed to higher temperatures. The different colors indicate the different elements in the sample but the same color should be used for both the line (theoretical amounts of one element) and the markers (experimental amounts of that same element). Colors are important to indicate different samples or different elements in the same sample and should be used to add clarity to the discussion of the data. The David Johnson lab (DCJ lab) primarily uses MagicPlot as its software of choice when figure making. The student version is free to download online and is user friendly to store and plot data.
15 Mike Pluth Lab Guide

Writing a paper in the Pluth Group

Preparation
- Make a folder in your shared Dropbox with the following folders:
  - Figures
  - Drafts
- Disable auto-compression in the main manuscript

During writing
- When writing:
  - Avoid editing directly in Dropbox to avoid file conflicts
  - Lab members should read and edit manuscript versions before sending to Mike
  - Communicate with Mike when to ask him to look at new things
  - Follow general formatting guidelines for target journal when relevant

Finalizing and Submitting
- Create the following files:
  - Endnote file (specify date of generation)
    Note: always be careful of journal endnote templates
  - Word file with suggested reviewers (name, email, and institution)
  - SI containing relevant data, including NMR spectra of all new compounds
  - Generate figures in Illustrator, and ensure that content is editable (i.e. text is editable text rather than vector lines). Save as compressed TIFF, and then resize in Photoshop. Make sure all files are editable, and that any linked images are in the shared Dropbox folder
  - Chemdraw figures do not need to be in Illustrator. Make sure to have a Chemdraw file in your Figures folder if you are using a Mac.
  - Print out all images to determine figure/table legibility
    - Consider font sizes, line weights, and colors
    - Images in manuscript draft should be sized to final journal sizes
    - Work on figures and schemes early and get feedback from other lab members. Think about the most concise way to display content. Your should strive to make the best figures possible
  - For revised manuscript, use the template for responding to reviewers in the Dropbox folder