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

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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:

Because your affiliations Gtf, Student	include:
- AND -	
You are using:	
Windows	~

You have access to the following software:

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

Microsoft Office 2016 for Windows	64-bit 32-bit
Microsoft Office 365	

Click on "Obtaining Software" link and follow instructions.

 Obtaining Software

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
 - o 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 **I** 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"

File	Home	Insert	Design	Transitio	ns Anin	nations	Slide Show	Review	View	Help
								✓ Ruler		
Normal	Outline	Slide	Notes	Reading	Slide	Handout	Notes	Gridline	S Notes	;
	View	Sorter	Page	View	Master	Master	Master	Guides		
	Pre	sentation Vi	ews			Master View	s	Show		۲ <u>م</u>

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.

	After				
Before	Click to edit Master text styles Second level				
Click to edit Master text styles Second level Third level	• Third level • Fourth level • Fifth level				
• Fourth level • Fifth level III iii 🐴 😘					
H12020 Footer	46 9/12020 Footer				

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.

Example 1	Example 2	
Click to edit Master text styles Second level Third level Fourth level Fifth level	Click to edit Master text styles Second level Third level Fourth level Ffth level	
	<#>	¢

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

AutoSave Off A Y Insert Design Transitions Animations EndNote X7 File Home Slide Show Review View Help 6 Colline Pictures 3D Models tə B S Add-ins ∽ 🚡 SmartArt Screenshot ~ Pictures Reuse Table Shapes lcons New Slide Slides Chart Noto Album Slides Tables Images **Recently Used Shapes** ⊠\\□0□∆lı⇔₽ß ⊌\\{}☆ Lines \\\ll%2232\G& Rectangles Basic Shapes ble Block Arrows ⎧╘གད๕ё३⇔़0;०;; ८२८८८०;०,०,०,०, D ∮∲∩ **Equation Shapes** ╋╼╳╬═₡ Flowchart Stars and Banners

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:
 - o Move to front
 - $\circ \quad \text{Move to back} \quad$
 - 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"



Animations	Slide Show	Review	View Help	EndNote X7	✓ Search		
					253	ΣŢ	🚛 Animation Pane
Fly In	Float In	Split	Wipe	Shape	Effect Options Y	Add Animation Y	🐓 Trigger 🗸
					Options	Animation	🏂 Animation Painter
	Animation				L2	Ad	vanced Animation

This will open up a menu on the right of the slide listing all of the animations on that slide. Using this pane, you can change the order of animations, as well as whether the animation starts "On Click" (will not appear until you click) or "Start with Previous" (will appear with previous object, allowing you to group that animation).



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."

Data	Review	View	Help	ρ	Search							
nnections		film Stocks	Geography	~	A↓ Z↓	Z A A Z Sort	Filter	Clear	Text to Columns	## *********************************	~	
s		0	Data Types				Sort & Filte	r		Data To	ols	

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."

onvert Text to Columns Wizard -	Step 1 of 3			?	~
he Text Wizard has determined that y	our data is Delimited.				
this is correct, choose Next, or choo	se the data type that be	est describes your dat	a.		
Original data type					
Choose the file type that best descri	ibes your data:				
Delimited - Characters s	such as commas or tabs	separate each field.			
 Fixed width - Fields are al 	igned in columns with s	paces between each f	field.		
Preview of selected data:					_
Preview of selected data:					_^
Preview of selected data:					^
Preview of selected data:					
Preview of selected data:				;	\ \ \ >
Preview of selected data:					\ \ >

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

Convert Text to Columns Wizard - Step 2 of 3								
This screen lets you set the delimiters your data contains. You can see how your text is affected in the preview b								
Delimiters Iab Semicolon Comma Space Qther:								
		\ ~						
Cancel < <u>B</u> ack <u>N</u> ext >	<u>F</u> inish							

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** [$\leftarrow \uparrow \rightarrow \downarrow$] 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-formulasbeginners/

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 Pls' 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:

	А	В	С
1	1	1	2
2	2	2	4
3	3	3	6
4	4	4	8
5	5	5	10
6	6	6	12
7	7	7	14
8	8	8	16
9	9	9	18
10	10	10	20

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.

Insert	Page La	yout Fo	rmulas	Data	Review	View	Help	Q	Search	
nended Ta ables	able	Fo Illustrations ~	Add- ins ~	Red	commended Charts		↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓	八 ~	Maps	PivotChart ~
			F 6	G	H Bubble	M ~ M	PivotCh			

A blank graph will appear. Right click on the graph and select "Select Data." A new window will pop up. Click **Add**.

Select Data Source	?	×
Chart <u>d</u> ata range:		Ť
Switch Row/Column		
Legend Entries (Series) Horizontal (Category) Axis Labels		
▲dd Image: Edit × Remove ✓ Image: Edit × Remove ✓ Image: Edit		
Hidden and Empty Cells OK	Ca	ancel

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 \uparrow

next to the "Series \underline{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 Xaxis). 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 <u>R</u>-squared value on chart."

Format Trendline								
Trendline Options V								
A A A A								
Logarithmi	c							
✓ ○ Polynomial	Or <u>d</u> er 2							
Po <u>w</u> er								
$\bigcirc \frac{M}{Average}$	P <u>e</u> riod 2 🗘							
Trendline Name								
<u>A</u> utomatic Linear (Sample 1)								
○ <u>C</u> ustom								
Forecast								
Eorward 0.0 periods								
<u>B</u> ackward	0.0 periods							
Set Intercept	Set Intercept 0.0							
✓ Display Equation on chart								
\checkmark Display <u>R</u> -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.

Resource: https://www.excelcampus.com/charts/chart-templates-default-formatting/

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-allyInapthalene). Follow this format for your file submisstion: 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
- Read the PDF installation guidelines: <u>http://hotwax.uoregon.edu/mnova/MestReNova_Installation_Instructions.pdf</u> (this should fix 99% of problems that come up during installation of MestReNova)
- 3. Follow instructions for downloading and installing MestReNova

Index of /mnova

	Name	Last modified	<u>Size</u>	Description
4	Parent Directory			
	MNovaQuickGuide.pdf	25-Oct-2019 10:44	166K	
?	MestReNova-12.0.4-22023.dmg	16-Sep-2019 11:41	164M	
?	MestReNova-12.0.4-22023.msi	16-Sep-2019 11:39	266M	
?	MestReNova-12.0.4-22023.x86_64.rpm	16-Sep-2019 11:41	208M	
?	MestReNova-12.0.4-22023_x64.msi	16-Sep-2019 11:39	252M	
F	MestReNova-12.0.4 Manual.pdf	25-Oct-2019 10:45	53M	
?	MestReNova-14.0.0-23239.dmg	16-Sep-2019 11:37	286M	
?	MestReNova-14.0.0-23239.msi	16-Sep-2019 11:35	371M	
?	MestReNova-14.0.0-23239.x86_64.rpm	16-Sep-2019 11:39	279M	
?	MestReNova-14.0.0-23239 x64.msi	16-Sep-2019 11:35	368M	
Ē	MestReNova-14.0.0 Manual.pdf	25-Oct-2019 10:44	54M	
F	MestReNova Installation Instructions.pdf	09-Oct-2019 15:15	170K	
F	MestReNova License Files.zip	09-Oct-2019 15:14	4.9K	
Ē	Mnova NMR Training for chemists on 1D and 2D NMR-Version 8.0.pdf	25-Oct-2019 10:44	4.2M	
?	mestrenova 12.0.4-22023 amd64.deb	16-Sep-2019 11:40	244M	
?	mestrenova 14.0.0-23239 amd64.deb	16-Sep-2019 11:40	364M	

Apache/2.2.15 (CentOS) Server at hotwax.uoregon.edu Port 80

2.3 Using MestReNova

<u>STEP 1</u> 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 \rightarrow Pages.



Open a file in MestReNova. Go to File \rightarrow Open \rightarrow Click and drag the folder from your experiment into MestReNova.

Pages				
	Favorites	Name	Date Modified V	
	Dropbox (Univer	1AGD019_o-tolyl3SiH_crude.fid.zip	 Today, 10:55 AM 	- 11
	All My Files	IAGD019_o-tolyl3SiH_crude.fid	 Today, 10:55 AM 	- 84
		3KEK034_analysis.mnova	 Yesterday, 5:12 PM 	
	Cloud Drive	3KEK034-02_more-dry_p-Me-allylbenz_1h_cdcl3.fid	 Yesterday, 5:11 PM 	- 84
	Applications	3KEK034-02_dried_p-Me-allylbenz_1h_cdcl3_bruker	 Yesterday, 5:10 PM 	- 84
	Deskton	3KEK034-01_p-Me-allylbenzene_1h_cdcl3	 Yesterday, 2:57 PM 	- 84
	- Booktop	3KEK094_analysis.mnova	 Yesterday, 2:56 PM 	- 84
3KEK094-01_p-CF3-al	lylbenz_1h_cdcl3	3KEK097_analysis.mnova	 Sep 1, 2020, 5:46 PM 	- 84
	O Downloads	3KEK097-08_org_pdt_1h_c6d6.fid	 Sep 1, 2020, 5:43 PM 	- 84
	Croative Cloud	SKEK094-02_p-CF3-allylbenz_19f_cdcl3.fid	Sep 1, 2020, 5:40 PM	- 84
	Creative Cibuu	3KEK094-01_p-CF3-allylbenz_1h_cdcl3	 Sep 1, 2020, 4:37 PM 	- 84
	Devices	3KEK097-06_t6_48h_1h_c6d6.fid	 Sep 1, 2020, 4:37 PM 	- 84
	Remote Disc	IKEK126_presentation_spectra.mnova	 Sep 1, 2020, 2:23 PM 	- 84
	0	IKEK126_HSiMe2Ph_analysis.mnova	 Sep 1, 2020, 2:23 PM 	- 84
	Media	3KEK096_analysis.mnova	 Aug 31, 2020, 9:08 AM 	- 84
	Music	SKEK097-01_DSiPh3_check_1h_c6d6	 Aug 31, 2020, 8:39 AM 	- 84
	150 Dhotoo	3KEK097-06_t5_on_1h_c6d6.fid	 Aug 31, 2020, 8:39 AM 	- 84
	IIII Photos	3KEK097-04_t2_5h_1h_c6d6.fid	 Aug 31, 2020, 12:10 AM 	- 84
	Movies	3KEK097-05_t2_7h_1h_c6d6.fid	 Aug 31, 2020, 12:10 AM 	- 84
	*	3KEK097-02_t1_1h_1h_c6d6.fid	 Aug 31, 2020, 12:10 AM 	- 84
	Tags	3KEK097-03_t1_3h_1h_c6d6.fid	 Aug 31, 2020, 12:10 AM 	- 84
		3KEK097-03_t2_3h_1h_c6d6.fid	Aug 31, 2020, 12:10 AM	
	New Folder O	Options	Cancel Open	I.
				1
				-11

STEP 2, continued

You should see a spectra. Now we need to set up your preferences to make your spectra more readable!



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 \rightarrow Select Font \rightarrow 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

1. You can change the color of the actual

Line width \geq 4.0 is recommended.

Under "1D"

the time.

$\bullet \odot \bullet$ Properties **—**, 🖽 Geometry NMR Spectrum Metadata General Show Baseline Grid Show Horizontal Show Vertical 뤴 1D Show Frame Scales Show Over Horizontal Light Gray Color: Line Width: 2.5 🚶 Peaks ∬ Integrals Multiplets Integrals **Fitting** Assignments Set as Default Restore ОК Cancel Apply $\bullet \odot \bullet$ Properties 🦢 , 🗄 Geometry NMR Spectrum Metadata spectra here. I prefer to use black most of General 2. Line width can be increased. This will help Style: Line ٢ with visibility, especially for presentations. 1D ~ Color: ▼ ^y_× Scales Line Width: 4.0 Horizontal Vertical Peaks Multiplets Integrals Fitting Resignments 2 Prediction Set as Default Restore OK Cancel Apply

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" \rightarrow "Horizontal" 1. Change the "Label" box to say " δ (\$u\$)"

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"

- 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!

	Properties							
— , 💾								
	Metadata Geometry NM	R Spectrum						
General	Integrals General							
Grid 1D	Color:	Green						
▼ ¹ / _× Scales	Line Width:	2.5	0					
Horizontal	🖸 Label							
Peaks	Font:	Arial						
Integrals	Decimals:	Select Font						
Multiplets	Position:	On Segment						
Fitting	Orientation:	Vertical	0					
Assignments	Show Calculation Metho	d Symbol						
2 Prediction	Curve	🛛 Range						
	Position: 30 %	C Margin: 3 %	0					
	Maximum Height: 40 %	0						
Set as Default Rest	pre	OK Cance						
	Set as Default Restore OK Cancel Apply							
Properties								
	Metadata Geometry NM	R Spectrum						
General	☑ Integrals General							
Grid	Color:	Green						
▼ ^{[Y} _x] Scales	Line Width:	2.5	0					
Horizontal	🖾 Label							
Vertical	Font:	Arial						
Integrals	Decimals:	Select Font						
Multiplets	Position:	On Segment						
Integrals								
Fitting	Orientation:	Vertical	0					
Fitting	Orientation: Show Calculation Methor	Vertical d Symbol	0					
الله Fitting الله Assignments الله Prediction	Orientation: Show Calculation Method	d Symbol	0					
Image: Weight of the second	Orientation: Show Calculation Metho Curve Position: 30 %	Vertical d Symbol © Range Margin: 3 %						
K Fitting 原 Assignments ② Prediction	Orientation: Show Calculation Methor Curve Position: 30 % Maximum Height: 40 %	Vertical d Symbol C Margin: 3 %						
H Fitting	Orientation: Show Calculation Methon Curve Position: 30 % Maximum Height: 40 %	Vertical d Symbol 0 Margin: 3 %	0					
Image: Construction Fitting Image: Construction Assignments Image: Construction Prediction	Orientation: Show Calculation Metho Curve Position: 30 % Maximum Height: 40 %	Vertical d Symbol C Range Margin: 3 %	0					
Image: Fitting Image: Construction Image: Construction	Orientation: Show Calculation Method Curve Position: 30 % Maximum Height: 40 %	Vertical d Symbol C Margin: 3 %						

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.





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 horizonal 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





If you want to quickly compare two spectra, use the stacking function in MestReNova.

Note: This is *not* ideal for presenting data formally. Select the spectra you want to stack and click on the "stack" button on the Pages toolbar.



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 ¹H 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 CDCl₃, you should take an NMR spectra of your product also in CDCl₃) unless solubility prevents this
- The AIST structural database has NMR spectral data for a wide range of common starting materials (<u>https://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi</u>)

2.5 Supplementary Resources

- Alternative MestReNova tutorial: <u>https://www2.chem.wisc.edu/~cic/nmr/Guides/Other/Mnova_NMR_Training_for_chemist</u> s on 1D and 2D NMR-Version 8.0.pdf
- Common NMR chemical shifts (¹H, ¹³C, ¹⁹F, ³¹P, ⁷⁷Se) organized by functional group: <u>https://organicchemistrydata.org/hansreich/resources/nmr/?index=nmr_index%2F1H_shi</u> <u>ft</u>
- Common ¹H NMR impurities (list of chemical shifts for solvents/common impurities for most relevant NMR solvents): <u>https://pubs.acs.org/doi/pdf/10.1021/om100106e</u>

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.



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

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
- 2. Follow instructions to download and install ChemDraw AND the necessary licenses

Chemdraw	Mac and Windows	-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 <u>download</u> page. - Use the second link to set up your account and the first link to refresh annually.	Available on computers in the Libraries	
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University of Oregon

Register for version 19.1.1, 18.X and 17.X

- ChemOffice Or ChemDraw 19.1.1, 18.X and 17.X
- Mnova ChemDraw Edition (included with ChemOffice Professional only)
 Register

Access version 16 and below, and Cloud Applications

- ChemOffice or ChemDraw version 16 and below
- ChemDraw Cloud (included with ChemOffice and ChemDraw Professional only)
- PerkinElmer Signals Notebook Individual Edition (for ChemOffice Professional only)
 Download
- 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 \rightarrow Apply Document Settings from \rightarrow ACS Document 1996



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 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.

View	Object	Structure	Text	Curve
✓ Show	Crosshai	ir	٦	сжх
✓ Show	Rulers			ж;
✓ Show	Main Too	olbar		
✓ Show	General	Toolbar		
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Show	Object T	oolbar		
Show	Analysis	Window		
Show	Chemica	Properties	Windov	v
Show	Info Wine	dow		
Show	Periodic	Table Windo	w	
Show	Characte	er Map Wind	ow	
Other	Toolbars			
Temp	lates			
Show	Chemica	l Warnings		
Show	Reaction	Interpretation	on	
Show	Docume	nt		೫/
Magn	ify			¥>
Redu	ce			Ж<

STEP 3a

Expand the space you have to work with

File \rightarrow Document Settings \rightarrow 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 \rightarrow Poster and increasing the height as needed or choosing Document Type \rightarrow Pages and increasing the number of rows.

Lavout	Document Type	1					
Header/Footer	Poster	Pages					
Drawing	Toster	Fages					
Text Captions	Document Size						
Atom Labels	Height: 10) in	Powe:	4	A Dages		
Property Labels	Theight. To	,	NOWS.	4	Fages		
Reaction Display	Width: 6.5	in	Columns:	1	Û		
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	Wargins						
	Left: 1 in	1	Right:	1 in			
	Top: 0.5	in	Bottom:	0.5 in			
	Page Overlap						
	Overlap: 0 i	n	🔽 Prir	nt Registration I	Marks		
	Dama Catur						
	Page Setup.	•					
Display Units: Incl	hes 🛕					Cancel	OK

STEP 3b

Increase the clarity of your bonds.

File \rightarrow Document Settings \rightarrow Drawing

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





Modified settings Increased line width to 0.015 in

e a loger loe	Drawing			
Layout	Chain Angle:		Bond Spacing:	
Header/Footer Drawing	120 🗘	degrees	18 🗘	O% of length
Text Captions			0.05 in	absolute
Property Labels	Fixed Length:	Bold Width:	Line Width:	
Reaction Display Colors	0.1574 in	0.0218 in	0.015 in	
	Margin Width:	Hash Spacing:		
	0.0175 in	0.02 in		
	Atom Indicators		Bond Indicato	rs



STEP 4



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 \rightarrow 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 \rightarrow 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.





*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.



Supplemental Information



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4 Igor Pro

Point Person: Tawney Knecht (<u>tknecht@uoregon.edu</u>)

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 colorcode 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
 - o 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:

1	А	В	С
1	Y_A	Y_B	X_WN
2	0	0	-15.3183
3	0	0	-15.2973
4	0	0	-15.2763

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+ \downarrow .

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:

🗽 lg	jor Pro 6	5.37									
File	Edit [Data	Analysis	Macros	Windows	Table	Misc	Help			
Table0:Y_A,Y_B,X_WN										×	
	Uni	used									
	Point		Y_/	A	Y_	В		X_WN			
		0		0			0	-15.3183			^
		1		0			0	-15.2973			
		2		0			0	-15.2763			
		3		0			0	-15.2543			
		4		0			0	-15.2333		 	
		5		0			0	-15.2113		 	
		6		0			0	-15.1903			
		7		0			0	-15.1693		 	
		8		0			0	-15.1473			
		9		0			0	-15.1263		 	
		10		0			0	-15.1043			× 1
<	_	_					_			 2)

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.

fultiple Selection p/Man Ticks Ticks	and Grids Tick Option	have more than one axis sele	ected ***	VI ive I Indate
o/Man Ticks Ticks	and Grids Tick Option			E Live opdate
		is Axis Label Label Option:	s Axis Range	
LogLin me Will change wave's units. an: am Margin	Axis Axis standoff Axis Thick: 2 Draw between	dirror Axis: No ticks ~ Axis offset 0 and 100 % of normal Praces	Font default Size: 20 Color Axis: V	Bold talic Underline Outline Shadow Set All to Axis Color
	Bar gap:	%	Axis Label: 🗾 🗸 7	Tick Label: 🗾 🗸
	LogLin ne Will change wave's units. in: im Margin	Axis standoff Axis standoff Axis standoff Axis standoff Control of the standof	Axis standoff Mirror Avis: No ticks Axis Thick: 2 Axis offset: 0 Draw between 0 and Wargin Control Draw on Top of Traces Category gap: % Bar gap: %	Axis standoff Mirror Axis: No ticks LogLin wow's units. Im Margin Bar gap: % Axis Label: 1 Axis standoff Mirror Axis: No ticks Axis offset 0 and Size: 20 Color Axis: 1 Axis Label: 1 Axi

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

		•		
Axis: Multiple Selec	ion V You have more than one axis selected ***	🗸 Live] Live Update	
Axis Auto/Man Ticks	Ticks and Grids Tick Options Axis Label Label Options Axis Range			
Auto Ticks Automatic Ticks Approximately: 5 Minor Ticks Minimum Sep: 10 Tick in center	Computed Manual Ticks Major tick marks Canonic tick: Canonic tick: Tick increment: Digits after dp: Minor ticks Number per major tick: Emphasize every:	s lect both a text war abels and a numi g tick locations. 	ve eric	
ModifyGraph mirror=2	Set to auto values minor=1,sep=10,fSize=20,axThick=2,standoff(left)=0			

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

Modify	Axis			?	×
Axis:	Multiple Se	lection V	*** You have more than one axis selected ***	🗸 Live U	pdate
Axis	Auto/Man Tic	ks Ticks and Grids	Tick Options Axis Label Label Options Axis Range		
• Ex	ponential labels Engineering Scientific	High trip: 10000 Low trip: 0.1 Exponent Prescale: 0	Tick Dimensions Grid: Off Location: Outside Style: Thickness Length Thickness Intervention Thickness Major Auto Auto Drew from Intervention	s: X Axis Line Thicknes: 0 100	B S %
Da	ate/Time Tick La Supp Time format Date format	bels ress date Normal ~ Short ~	Minor Auto Auto Color 5th Auto Auto Style: Subminor (log) Auto Auto Zero Line Thick:	Auto	
Modi	fyGraph mirro	r=2,minor=1,sep= Cmd Line	10,fSize=20,axThick=2,standoff(left)=0 To Clip Help		Cancel

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

odify Axis					?	×
xis: Multiple Selection 🗸	*** You hi	ave more tha	n one axis selec	ted ***	Liv	e Update
xis Auto/Man Ticks Ticks and Gr	ids Tick Options	Axis Label	Label Options	Axis Range		
Enable/Inhibit Ticks Enable ticks between Hinf Inhibit ticks:	and inf			Tick Label Thou Zero No tr Tick No U Units	Tweaks is ands separator is '0' ailing zeros aading zero Unit Prefix is Expone Inits in Tick Labels in Every Tick Label	ent
lodifyGraph mirror=2,minor=1,se	p=10,fSize=20,	axThick=2,	standoff(left)=	0		
Do It To Cmd Line	To Clip				Help	Cance

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

Modify Axis		?	\times
Axis:	left V	🗹 Live Upd	date
Axis Auto/M	an Ticks Ticks and Grids Tick Options Axis Label Label Options Axis Range		
Insert	Auto Labort		
Font	Axis Label IZ20Abcothanco (A III)		븟
Font Siz	ze V		Ç
Units	▼	>	
Specia	al 🔻 Label Preview		_
Trial Expon O Zero O Six	Absorbance (A.U.)		
ModifyGraph Label left "\Z Label bottom	mirror=2,minor=1,sep=10,fSize=20,axThick=2,standoff(left)=0;DelayUpdate 20Absorbance (A.U.)",DelayUpdate "\/Z20"		~
Do It	To Cmd Line To Clip He	dp C	ancel

odify	Axis		?	×
xis:	bottom	~	🗸 Live U	Ipdate
xis	Auto/Man Ticks	Ticks and Grids Tick Options Axis Label Label Options Axis Range		
In	sert			
	Font -	Axis Label		
		\Z20Wavenumber (cm\S-1\M\Z20)		^
L.	Font Size			\sim
	Units 🔻	<		>
	Special 🔻	Label Preview		
-Ті (rial Exponent Zero	Wavenumber (cm ⁻¹)		
(• Six			
lodi	e) Six ifyGraph mirror=2 el left "\\Z20Absor el bottom "\\Z20N	minor=1,sep=10,fSize=20,axThick=2,standoff(left)=0;DelayUpdate bance (A.U.)",DelayUpdate avenumber (rm)\S.11\MU?20)"		
lodi abe	●) Six ifyGraph mirror=2 el left "\\Z20Absor el bottom "\\Z20W	minor=1,sep=10,fSize=20,axThick=2,standoff(left)=0;DelayUpdate bance (A.U.)";DelayUpdate avenumber (cm\\S-1\\M\\Z20)"		

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 superscripts 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

Modify Axis	?	×
Axis: Multiple Selection V Max You have more than one axis selected max	🗸 Live	Update
Axis Auto/Man Ticks Ticks and Grids Tick Options Axis Label Label Options Axis Range		
Labels On V		
Label Position Mode: Compatibility ~ Axis label rotation 0	~	·
Axis label margin: 0 Tick label rotation 0	v	·
Axis label position: 0 Tick label off	set 0.00	
Axis label lateral offset: 0		
ModifyGraph mirror=2,minor=1,sep=10,fSize=20,axThick=2,standoff(left)=0;DelayUpdate Label Heft "I\Z20Absorbance (A.U.)",DelayUpdate Label bottom "\\Z20Wavenumber (cm\\S-1\\M\\Z20)"		~
Do It To Cmd Line To Clip He	əlp	Cancel

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

Modify	Axis						? ×
Axis:	left	~				V Liv	ve Update
Axis Auto U Z	Auto/Man Ticks sscale Settings Reverse axis lse data limits ero isn't special Autoscale Only Vir	Ticks and Grids	Tick Options	Axis Label Label C tanual Range Settings Numeric Manual Min 0 Manual Max 45 Expand 5%	Pptions Axis Hange	Quick Set	
Modif Labe Labe SetA	fyGraph mirror=2 I left "\Z20Absor I bottom "\Z20W xis left 0,45	2,minor=1,sep= /bance (A.U.)"; /avenumber (cr	10,fSize=20, DelayUpdate n\\S-1\\M\\Z2	,axThick=2,standof 20)";DelayUpdate	f(left)=0;DelayUpc	late Help	Cancel

Modify Axis	? ×
Axis: bottom 🗸	Live Update
Axis Auto/Man Ticks Ticks and Grids Tick Options Axis Label Label Options Axis Range	
Autoscale Settings Manual Range Settings Reverse axis Manual Min Use data limits -15 Zero isn't special Manual Max 7 Expand 5%	Quick Set Y_A Y_B X_WN Y Min/Max X Min/Max Full Scale
ModifyGraph mirror=2,minor=1,sep=10,fSize=20,axThick=2,standoff(left)=0;DelayUpdate Label left "\Z20Absorbance (A.U.)";DelayUpdate Label bottom "\Z20Wavenumber (cm\\S-1\\M\\Z20)";DelayUpdate SetAxis left 0,452DelayUpdate SotAxis bottom _15_7 Do It To Cmd Line To Clip	Help Cancel

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:

Modify Trace Appearance		? ×
Trace	Mode	
Y_A Y_B	Lines between points	
		Color: Set as f(z)
Line Size: 2.00	Grouping: None	✓ Hide Trace
Style: 0 ~	Error bars Gaps	
ModifyGraph Isize=2,rgb(Y_A)=(0,0,0),rgb(Y_B)=(522	224,0,0)	$\hat{}$
Do It To Cmd Line	To Clip	Help Cancel

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:

Modify Graph	?	\times
Margins: Left Auto Bottom: Auto Right Auto Top: Aut	to	
Width mode: Aspect ~ 1.2 * height		
Height mode: Absolute ~		
Units: inches ~ Magnification: None	~	
Swap X and Y Axes Marker size: Auto		
Graph font: default ~ Font size: Auto		
ModifyGraph width={Aspect, 1.2},height=288		$\hat{}$
Do It To Cmd Line To Clip Help	Can	cel

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. I

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:

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:

Search Add Annotation	?	\times
Annotation: TextBox v Name: text0		
Text Frame Position Symbols Tag Arrow ColorScale Main ColorScale Axis Labels ColorScale Ticks		
EditText Y Annotation		
Insert		^
Dynamic 💌		
Font 👻		
Font Size 💌		
Del Festóles		~
Kei. Font Size		>
Adi, Line Spacing: 0.00		
	Preview	~
	Do It	
	To Clip	р
	To Cmd	Line
	Help	
	Cance	el 🛛

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:

🔄 Add Annotation		?	×
Annotation: Leger	nd V Neme: text0 Symbols Tag Arrow ColorScale Main ColorScale Axis Labels ColorScale Ticks		
EditText ~	Annotation		
Insert: Dynamic Font Font Rel. Font Size	\s(Y_A)Y_A \s(Y_B)Y_B <		>
Special	Adj. Line Spacing. 0.00	Preview	
	— Y_A — Y_B	Do It To Clip To Cmd L) Line
		Help	
		Cance	1

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:

الا Add Annotation	? ×
Annotation: Legend V Name: text0 Text Frame Position Symbols Tag Arrow ColorScale Main ColorScale Axis Labels ColorScale Ticks	
EditText Y Annotation	
Insert Dynamic V Font V Font Size V	Î
Special Adj. Line Spacing: 0.00	>
Sample A Sample B	Preview V

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."

Save Graphics File	? ×
Size: Same Ocustom Width: 6.416667 Height: 5.291667	inches \sim
Format	
TIFF File V	
Color Resolution: 8X Screen ~	
● RGB ○ CMYK	
File:	
Name: Graph0.tif Path: _Use Dialog_	~
Force Overwrite	
Path:	
SavePICT/E=-7/B=576	
Dolt To Cmd Line To Clip He	lp Cancel

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."

			Graph Misc Help				
			Append Traces to Graph	Í			
			Append to Graph	>			
			Modify Graph Frame Modify Trace Appearance Reorder Traces Replace Wave Modify Contour Appearance Modify Image Appearance	>			
			Set Axis Range Autoscale Axes Label Axis Modify Axis	Ctrl+A			
			Add Annotation Add Controls Select Control	>			
			Show Info Show Tools Show Trace Info Tags	Ctrl+I Ctrl+T Ctrl+Alt+I			
			Capture Graph Prefs	7			
Capture	Graph Pre	eferences	Packages	>		2	×
							~
	default	Window Posi	tion and Size				
	default	Page Setup					
	default	ShowTools, S	ShowInfo, and Cursors				
		🖂 Margins, Heig	ght and Width Modes				
		Background (and Graph Colors				
		🔽 Font, Font Siz	e, and Font Style				
		XY Plots: Axe	s and Axis Labels				
		XY Plots: War	ve Styles (lines, markers,	colors,)			
	default	Category Plo	ts: Axes and Axis Labels				
	default	Category Plo	ts: Wave Styles				
	default	🗸 Image Plots: /	Axes and Colors				
	default	Contour Plots	Axes, Levels, Colors, La	bels, Updates			
	Capture F	Prefs	Revert to Defaults		Help	Cancel	

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 \rightarrow Procedure Windows \rightarrow 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 \rightarrow 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 \rightarrow Graph Macros \rightarrow *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:



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.



Closeup



5.3 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: <u>https://casit.uoregon.edu/faq/overview-of-adobe-creative-cloud-application</u>
- 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 <u>File</u> menu and clicking <u>New Document</u>. 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.

Nar	ne: My Example Docum	ent	
Prof	ile: [Custom]		
Number of Artboar	ds: ≑ 1	3월911 -	
Spaci	ng: - 20 pt	Columns:	÷1
Si	ze: [Custom]		
Wid	th: 500 pt	Units:	Points
Heig	ht: 500 pt	Orientation:	✓ Points Picas
Ble	Top Bott ed: 💠 0 pt 🛟	om Left O pt 🗘 O pt	Inches Millimeters
▼ Advanced			Centimeters
Color Mo	de: CMYK		Pixels
Raster Effe	ts: High (300 ppi)		
Preview Mo	de: Default		
	Align New Objects	s to Pixel Grid	

Image 1. New Document configuration dialog box.

Editing the document preferred *Units* can be accomplished by the shortcut Clt+K or by navigating the <u>Edit</u> menu to <u>Preferences</u> and <u>General...</u> (image 2). Once at the Preferences dialogue box navigate to the <u>Units</u> tab change the preferred *Units* (image 3).

My Settings	+		
Sync Settings	÷-		
Preferences	•	General	Ctrl+K
		Sync Settings	
		Selection & Anchor Dis	alav

Image 2. General Preferences menu navigation.

Preferences					
Preferences General Sync Settings Selection & Anchor Display Type Units Guides & Grid Smart Guides Slices Hyphenation	Units General: Stroke: Type: East Asian Type:	Points Points Points Points	a a but Units Are Points	5	
Hyphenation Plug-ins & Scratch Disks User Interface File Handling & Clipboard Appearance of Black GPU Performance	Identify Objects By:	Object Name	XML ID		
				ок	Cancel

Image 3. The Units tab in the Preferences dialog box.

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 <u>File</u> menu to <u>Document Setup...</u>. On the Document Setup dialogue box click <u>Edit Artboards</u> to access the editor (image 4).



Image 4. Document Setup dialog box.

The <u>*Edit Artboard*</u> 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.



Image 5. The Artboard editor.

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 6. (Left) Upper right point of square selected with Selection Tool (Center) Upper right point of square selected with Direct Selection Tool (Right) Selection Tool and Direction Selection Tool menu icons.

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 <u>File</u> menu to <u>Layers</u>. 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.

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.



Image 8. Notice that all the blue circles are hidden and also the medium red square. Since the small red square is selected, the Squares Layer and Small Sub-Layer exhibit the small blue 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.

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).



Image 10. Second half of the Control bar.

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 <u>*Effect*</u> menu to the <u>3D</u> option and select <u>*Revolve...*</u>. (Image 13) In the Revolve menu (Image 14), make sure the <u>*Preview*</u> box is checked (Red arrow). Moving the box changes the angle of rotation about the axis.

elect	Effect	View	Window	Help				
	Apply Last E	/ Last Ef Effect	fect		B第① B第①ブ	Adobe Illus	strator 2020	
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U Previe	Illustr	ator Effe	ects					
	3D				►	Extruc	de & Bevel	
	Cor	overt to	Shape		•	Revol	/e	
	Cro	p Marks				Rotate	9	
	Dist	tort & Tr	ansform		•			
	Patl	h			•			
	Patl	hfinder			►			
	Ras	terize						
	Styl	lize						
	SVO	3 Filters						
	Wai	rp						
	Photo	shop Ef	fects					
	Effe	ect Galle	ry					
	Arti	stic			►			
	Blu	r			►			
	Bru	sh Strok	ces		•			
	Dist	tort						
	Pixe	elate			►			
	Ske	tch						
	Styl	lize			•			
	Tex	ture			•			
	Vide	eo						

Image 13: Navigate to the Revolve button

		3D Revolve Options
	Position: Off-Axis Front	
		 → ○ -18° ↓ ○ -26° → ○ 8°
		Perspective: 0° >
	Revolve	
-	Angle: 🔶 360°	Cap: 💿 💿
	Offset: 0 pt > from	Left Edge 🗸
	Surface: Plastic Shading ~	ave occurred.
	Preview Map Art	(More Options) Cancel OK

Image 14: Revolve menu. The rotation axis and angle can be manually changed, or click and drag on the box. Note when adjusting coloring and transparency the surface shading will also affect color and appearance.

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).



Image 15: A 3D shape created using Revolve rotated 90°. Rather than rotate the whole shape, the new triangle shape is revolved about the new center axis.

To fix this, the 3D shape must be expanded. Select the shape, navigate to the <u>Object</u> menu and select <u>Expand Appearance</u> (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.

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 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 <u>*Window*</u> menu to the <u>*Stroke*</u> 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).

44 X
\$Stroke Gradient Transparency ▼ ≣
Weight: 🗘 1 pt
Cap: ICC
Corner: 🔽 🚰 🚰 Limit: 10 x
Align Stroke: 📙 🔚 🔚
Dashed Line
dash gap dash gap dash gap
Arrowheads: 🗾 🔻 🗾
Scale: 100% 100%
Profile: Uniform 💌 D.K 🔛

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.



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).

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 24. Example of text warp using the flag preset.

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 <u>Window Menu</u> to <u>Type</u> and then <u>Character</u>. 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).



Image 25. The Type Character dialogue box before and after "show options".

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 <u>Object</u> menu to <u>Clipping Mask</u> and selecting <u>Make</u> (image 26).



Image 26. Navigating to the Clipping Mask Make button.

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.

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 <u>*Release*</u> option directly below <u>*Make*</u> in the <u>*Object*</u> menu.



Image 28. By double clicking any object within a clipping mask the user will be able to edit the location of objects within the clipping mask.

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 vectorbased 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).



Image 29: Exporting a figure as a vector image

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)

		SVG Options	
I	Styling:	Internal CSS	✓
	Font:	Convert To Outlines	• —
	Images:	Preserve	~
	Object IDs:	Layer Names	~
l	Decimal:	2	
	l	🗌 Minify 🗌 Responsive	
	Show Code	e 🔇 Cancel	ОК
			_

Image 30: SVG save options

- 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 <u>Type</u> menu and select <u>Create Outlines</u>



Image 31: Type menu bar

- \circ $\,$ Make sure the original .ai file is larger than the size you want in your word doc
- Expand again (Image 32)



Image 32: Expand menu

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 <u>Edit</u> menu to <u>Preferences</u> and then <u>Smart Guides...</u> (image 33). It can be useful to lower the *Snapping Tolerance* when working with very detailed sets of objects.



Image 33. Smart Guides tab in the Preferences dialogue box.

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 <u>View</u> menu to <u>Rulers</u> and <u>Show</u> <u>Ruler</u> (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 <u>View</u> menu to <u>Guides</u> (green arrow).



Image 34. Creating and editing user created Guides.

Grid Alignment

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



Image 35. Navigating to Guides and Grid... – notice the grid in the background.

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).

Preferences	
Preferences General Sync Settings Selection & Anchor Display Type Units Guides & Grid Smart Guides Slices	Guides & Grid Guides Color: Cyan Style: Lines
Hyphenation Plug-ins & Scratch Disks User Interface File Handling & Clipboard Appearance of Black GPU Performance	Color: Black Style: Lines Gridline gvery: 50 pt Subgivisions: 10 Subgivisions: 10 Grids In Back Show Pixel Grid (Above 600% Zoom)
	OK Cancel

Image 36. Guides and Grid tab of the Preferences dialogue box.

6 CrystalMaker

Point person: Tawney Knecht (<u>tknecht@uoregon.edu</u>)

6.1 Download Information

- Go to <u>https://researchguides.uoregon.edu/chemistry/software</u> 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, <u>annie@uoregon.edu</u>

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

Video Tutorials Learn about CrystalMaker X in these detailed audio-visual tutorials						
Introduction:						
Overview	Interface Tour	The Structures Library	What's New in 10.4?			
Basics:						
Building a New Crystal	Building a New Molecule	Atomic Radii & Colours	Selection Tools			
Measurement	Annotation	Seeing Your Structure in 3D	Preferences			
Advanced:						
Lattice Planes	Working with Molecular Crystals	The Distance Explorer	Visualizing a Cluster			
Showing Cavities	Building Massive Polyhedra	Volumetric Data	Creating a Domain Boundary			
Placing a Molecule Into a Crystal	Using the Leap Motion Controller	Creating an Animation	Visualizing a Trajectory			
Diffraction	Live Powder Diffraction	Live Intensity Mode (10.5)				

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 (<u>https://icsd.products.fiz-karlsruhe.de/</u>) and click on "LOGIN to ICSD" in the top right corner of the screen. This should bring you to this page:

¢ _{ICSD}		We	lcome to ICSD Web.	IP authenticated	d (128.223.93	.176). Univ Oregon				FIZ Change Passwo	Karlsruhe C rd Close se	ontact ssion
Login	Basic Search &	Retrieve							0	Search Action		
LoginId:	Free Text Search	1								Run Query	Clear Qu	lery
Password:	General Attributes									Search Summary		
Login Personalized	Bibliography									Basic Search:		-
Lost Personalize password? account	Authors						Year of Publicatior			Query History		
Content Coloritor	Title of Journal									Number of querie	95:	0
Experim inorganic structures	Title of Article									Clear Qu	ery History	
Experim. metal-organic str.												
Theoretical structures	Composition	Ca 0			Poriodic	Table	Number of	2				
Navigation	Composition	660			Fellouid	Table	Elements	2				
Q Basic search & retrieve	Cell											
	Cell Parameters											
Advanced search & retrieve	Cell Volume						Tolerance	+/-	%			
Q Bibliography	Symmetry											
Q Cell	Space Group		Space Group									
Q Chemistry	Symbol		Number									
Q Symmetry	Crystal System	-	Centering		-							
Q Crystal Chemistry	Exp. Info. & Ref. I	Data										
Q Structure Type	New Data Only											
Q Experimental Information	PDF Number			Tem	nperature			K •	-			
Q DB Info	ICSD Collection											
Q Expert Search	Code			Pre	ssure			MPa •	•			
Query Management												
Manage Queries		Clear Basic	Search			Count Basic Search						
List Combined Queries												
👍 Create Combined Query												
ICSD links												
C ICSD News												
C ICSD Questionnaire												

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.

G ICS	SD		Welcome to ICSD Web. IP authenticated (128.223.93.176). Univ Oregon					FIZ Karlsruhe Contact Change Password Close session		Contact session
Results: L	_ist View							# of Hits: 8	32 (1 sele	cted) 💡
Q Back	to Query Q Show	Detailed View	🖺 Export [Data 🖶 Print 🖌	Visualize Structure	✓ Visualize Powder Pa	ttern 💌	Column Select	ion	Filter
	HMS ≎	Struct. Form. \$	Struct. Type \$	Reference \$	Temperature \$	Pressure \$	Calculated Density ≎	Measured Density \$	₽.	
	F m -3 m	Ce O2	Cu2Se	Applied Physics Letters	1770.00	0.101325	6.82		\$	*
~	Fm-3m	Ce O2	Fluorite#CaF2	Journal of Solid State C	293.00	0.101325	7.21		\$≯-	*

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

→ ■ ● ■ ● ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■	o ar Tidy	() O∕∖nt Ro	🗩 🕂	Annotate	Ad
View Direction	U	V 1 tice Vector: ne Normal:	W 1 [UVW] N(hkl)	d v	
Constrain ve	rtical dire	ection			
a a*	b b*	с с*	[1 1 0]	[1 0 1]	
2			OK	Cancel	

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

72155 - CrystalMaker Education Edition						
Mod	el	Transform	Calculate	Window	Help	
~	Ba	all & Stick		Ctrl	+1	
	Space Filling			Ctrl+2		
	Polyhedral			Ctrl+3		
	Wire Frame			Ctrl+4		
	St	ick		Ctrl	+5	
	EI	lipsoids		Ctrl	+6	

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

Scale Centre	Re ^r r	(e Cluster	O Tidy	Orient Ro
Axial Range Limits:				
min		max		
x: 0.0	÷	1.0	÷	1.0 ~
у: 0.0	÷	1.0	÷	1.0 ~
z: 0.0	÷	1.0	÷	1.0 ~
🕀 Expand Rang	ge		Add	Cells
Contract Ran	ge		Remov	e Cells
Reset Range	5		Cell Co	ntents

- Turn your structure into a cluster or nanocrystal by clicking on Cluster.
 - Enter in your central atom
 - o Enter in the desired radius
 - o Click "Reset Cluster Size"

→ (tre F	ange Clr^ter	Tidy Orient F
Define s	pherical cluste	er:
Centre:	Ce1 Use centre	v e of selection
	Inner	Outer
Radius:	0.0 Å 🗘	6.0 Å 🗘
	Reset Clu	ster 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:



- 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...



- To change bond type, click on the X 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

File	Edit	View	Model	Transform	Calculate	W	/indow	Help			
	New Window Ctrl+N New Window with Structure							L D Axes Cell	Scale	- Centre	
	Open Open Open	 Recent with Fc	ormat	C	itrl+0	• •	4		2	111	0
	Add t Save	o Wind	ow	C	itrl+S	۲					
	Save . Expor	As t Data		C	trl+Shift+S	×			_	,	
	Expor	t Graph	ics			۲		2D Graphics	s	Ctrl+	G
	Expor Close	t Video				•		COLLADA 3 STL 3D File	D File		

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: <u>https://researchguides.uoregon.edu/chemistry</u>

7.1 Software

- Avogadro
- Crystallography
 - o Mercury
 - o GSAS
- Dropbox
- Figures
 - o GIMP
 - o Inkscape
- Graphing
 - Origin Pro
 - o MagicPlot
- ImageJ
- Reference managers (specific ones may be preferred by some labs)
 - o Endnote
 - o Mendeley
 - o 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): <u>https://icsd.products.fiz-karlsruhe.de/</u>
- NIST Chemistry Webbook: <u>https://webbook.nist.gov/chemistry/</u>
- Scifinder:

https://scifinder.cas.org/

- Spectral Database for Organic Compounds (SDBS): https://sdbs.db.aist.go.jp/sdbs/cgi-bin/direct frame top.cgi
- Web of Science:
 <u>https://apps.webofknowledge.com/</u>

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
- 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:

lgor:

- 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\F'Symbol'q \F'Arial'(°) *The degree symbol is 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.

10 Amanda Cook Lab Guide

Cook Lab Software Summary

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).



How to Present NMR Data (and spectra in general)



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
 - o Avogadro
 - Mercury (x-ray structures)
 - o Vesta
 - o 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
 - o 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
 - o 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 A is good for tubes, 3 A makes a CPP)

	n: 6 🜩	Length: 15.00 🜩	Cap with hydrogen
3.	m: 5 🜩	Unit: angstrom 🔻	Find double bonds

- 4. Do not minimize, save as a .mol file
- 5. Open in ChemDraw and orient to preferred perspective using the Structure Perspective tool
- 6. Flatten the molecule and ensure all front bonds are in the front and back bonds are in the back
- 7. 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
 - $\circ \quad \text{For figure creation} \quad$
- Matlab
 - $\circ \quad \text{For data analysis} \\$
- CiscoConnect
 - \circ $\,$ 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 labrelated or not
- Lab business and safety
 - o 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

<u>Subgroup (~1 hour, once per week)</u>

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.
14 David Johnson Lab Guide

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



Figure 1: In-plane x-ray diffraction as a function of temperature. Example of a DCJ lab

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

	Word Options	Compress Pictures
General Display Proofing	Keep bullets and numbers when pasting text with Keep Te Add control characters in Cut and Copy Use the Insert key for paste	Compress pictures to reduce the size of this file.
Save	Show Paste Options button when content is pasted	Picture Quality: Use Original Quality
Typography	V Use smart cut and paste U Settings	✓ Delete cropped areas of pictures
Language	Image Size and Quality Document1 v	
Advanced	Discard editing data ⁽¹⁾	Apply to: • All pictures in this file
Customize Ribbon	Do <u>n</u> ot compress images in file ①	 Selected pictures only
Quick Access Toolbar	Set default target out <u>p</u> ut to: 220 ppi	
Add-ins	Chart Document1 V	Cancel
Trust Center		

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