

Instructions

Instructions:

It is great if you read this document before the lab meeting, but do not complete this assignment until you are in the lab with your instructors.

1. When you are in lab and ready to collect data, **use the instrument computer** to [make a copy \(click\)](#) of this file in the Advanced Lab Google Drive folder by clicking on the link here [\(click\)](#).
2. **Change the file name:** change “NAME” to your Group Name.
3. Notice that there are multiple tabs to this google doc shown in the left hand table of contents. If you don't see the tabs, expand the table of contents using the icon on the top left of this window, under the top toolbar:  4
4. Click “**Share**” in the upper right corner and each member of the group should share it with their gmail address with “Editor” privileges.
5. Using your own computer, logged into your own google drive account, organize this file by placing it into the Drive folder for this class. (My Drive > Classroom > Physical Chemistry Lab)
6. Assign leading roles for each person, for example some suggested roles are:
 - a. **Figure Fairy** - ensures all figures are clear and captions are written well and numbered accordingly.
 - b. **Table Czar** - ensures all tables are complete and that titles and figure numbers are appropriate.
 - c. **Wordsmith Wonder** - describes what was done in clear, precise language.
 - d. **Significance Hero** - checks that values are reported with reasonable precision.
7. As a group, record your work, including major steps, instruments used, their settings, and the data collected. All members of the group should work together to create a complete record of the lab work and the data.
8. After the Group Notebook is complete, Copy/Paste the data into the appropriate tab in your Individual Notebook template – the individual notebook template should already be in your google drive in My Drive > Classroom > Physical Chemistry Lab.

Part I Group Notebook

Group ELN – Absorption Spectrum of Conjugated Dyes, Part I

Due by end of meeting

[Put Group Name Here]

[Put Date Here]

Member Name 1

Member Name 2

Member Name 3

Member Name 4

Spectrum of Conjugated Dyes, The Particle in a Box (PIB) Model

Experimental Materials, Methods, and Data:

Instrument:

Type of Instrument:	UV-visible spectrometer
Manufacturer:	Agilent
Model:	
Tolerance:	
Accessories Used:	
Validation Test:	

[DESCRIPTION OF INSTRUMENT: *An example is provided here for reference – please replace this text with your own experimental plan. Please note that some of the information below about the instrument is outdated.* UV-vis spectral data were collected using a Cary 1G UV-Vis spectrometer for this experiment. The tolerance in wavelength reported by the manufacturer is ± 0.2 nm. The instrument wavelength calibration was validated using holmium oxide (Ho_2O_3). The resulting spectrum and validation analysis is given below.]

A. Validation Spectrum (place holder)

[FIGURE: *Insert and image of the validation spectrum or spectra here Provide a statement about the instrument validation before the figure (see example) – did it work and what does it tell you? Place a caption below the figure to tell your reader what it is at a glance.*]

Figure 1: [Put a descriptive caption here. eg “Holmium Oxide Validation spectrum” would be appropriate if you used holmium oxide to do the instrument validation. Figure headings/captions are placed BELOW the figure and are numbered in consecutive order.]

Table 1: [Table headings always come BEFORE the table. Put a brief descriptive heading here.]

A. Validation Data Table (place holder)

[TABLE: *Copy and paste the results of the validation peak searching – format it so that it is easy to read. Provide a descriptive title above the table.*]

Instrument Settings for Data Collection:

[Comments; indicate dye name, solvent, cell type, how samples were prepared for data collection.]

NOTE: The Data Interval setting is a factor in determining the experimental uncertainty in peak wavelength.

Table X: [Table headings always come BEFORE the table. Put a brief descriptive heading here.]

Scan Range:		Dwell Time:	
Data Interval:		Scan Speed:	
Other Details:			
File Directory and Root File Name:			

Sample Preparation:

[Comments; indicate dye name, solvent, cell type, how samples were prepared for data collection.]

Table X: [Table headings always come BEFORE the table. Put a brief descriptive heading here.]

<i>File #</i>	<i>Comments (# drops, approx absorbance, max wavelength)</i>
1	
2	

Overlaid Spectra of Four Dyes:

B. Overlaid Spectra of Four Dyes (place holder)

[FIGURE: Place an image file of the overlaid spectra of the four dyes here. The wavelength of maximum absorbance should be labeled on each spectrum, and each spectrum should be labeled with its Dye name (it is fine to use labels like Dye 1, Dye 2, Dye 3, Dye 4 as long as these abbreviations are defined elsewhere.) The figure should be preceded by a brief description and a title and caption should be placed directly following the image.]

Figure X: [Use the correct number and give a descriptive caption for this figure]

Table X: λ_{\max} values (include all class data).

Team	Dye 1 λ_{\max} (nm)	Dye 2 λ_{\max} (nm)	Dye 3 λ_{\max} (nm)	Dye 4 λ_{\max} (nm)
Team 1				
Team 2				
Team 3				
Team 4				
Mean \pm Stdev.				
Literature Value				

Evidence for the effect of concentration on the spectrum:

C. The effect of concentration on the spectrum (place holder)

[FIGURE: Place an image file that provides evidence as to the effect of concentration on the spectrum of a dye molecule. The lambda max should be labeled for each spectrum. The dye name and approximate difference in the concentrations should be indicated in the figure caption (eg the spectrum with a stronger absorbance is twice as concentrated as the other.)

Figure X: [Use the correct number and give a descriptive caption for this figure]

Evidence for the effect of mixing on the spectrum:

D. The effect of mixing on the spectrum (place holder)

[FIGURE: Place an image file that provides evidence of the effect of mixing on the spectrum of dye molecules. The lambda max should be labeled for each spectrum. The dye name and the approximate difference in the concentrations should be indicated in the figure caption (eg the spectrum with a stronger absorbance is twice as concentrated as the other.)

Figure X: [Use the correct number and give a descriptive caption for this figure]

Computational Methods and Data:

Method:

Prediction of Theoretical Absorption Maxima Using Particle In The Box Model– The particle in the box model was applied to the series of dyes to predict their theoretical absorption maxima (λ) using Equation 1:

$$\lambda = \frac{8mca^2}{h} \frac{(P+3+\gamma)^2}{P+4} \quad (1)$$

Where [*..describe what each variable is*].

For each dye, the theoretical absorption maximum (λ) was calculated using the dye's specific P-value and a range of candidate γ values from 0 to 2 in increments of **0.01**. The residual for each dye was determined as the

relative difference between the experimental absorption maximum and the calculated theoretical value. The residuals were summed across all dyes in the series for each candidate γ value.

The γ value that minimized the total residual sum was identified as the optimal correction factor for the homologous series. This process was implemented in MATLAB to systematically compute and minimize residuals, yielding an optimized γ value for the dye series.

Computational Data:

The PIB model and MatLab were used as described above to find an optimum gamma (γ) value and then to calculate theoretical wavelengths of maximum absorbance:

[Notes and information about what was input into MatLab - could be in form of a table]

[paste a title and caption for the table here, if appropriate]

Paste MatLab output here
(place holder)

[paste the output from the dye_v4_beta script here]

Residuals vs Gamma of 4 Dyes
(place holder)

[FIGURE: Place the residuals plot here, and add a title and caption below the figure.]

Figure X: [Use the correct number and give a descriptive caption for this figure]

References:

Reference any outside source material used using a citation manager and ACS style citation formatting (superscript citation numbers in text, endnotes).

Submit this group ELN during the lab meeting. Then, complete the relevant sections of the Individual ELN with the remaining time. Any work that is not completed during the meeting is due before the next meeting or according to the syllabus schedule.