Exam 2, Q1 (4/1/20, Sturgeon)
Chem 322: Quantum Mechanics (30 pts total)
Material Covered: Chapter 5 (Engel, 2nd Ed.)

Name _____
(please print)

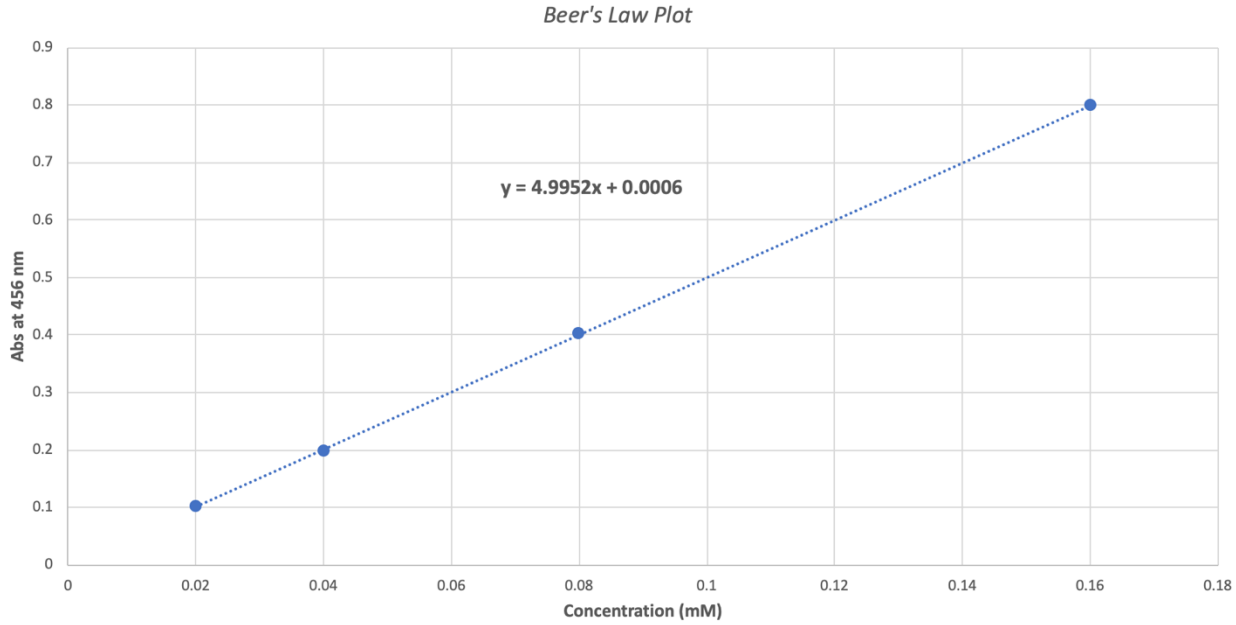
Exam instructions: This is question 1 of 3 for your "take-home" exam. Question 2 will be available on Thurs and question 3 will be available on Friday. During this exam, you may use your textbook, lab notebook, class notes, and/or any other documents you prepared. ***This question is due by 5 pm TODAY…please take a picture/scan and email them to me.***

I agree to follow the guidelines listed above and state that I have neither given nor received any unauthorized aid on this exam.

_____ (*signature*)

---

1) UV-Vis spectroscopy is initially presented in the undergraduate curriculum as a tool to determine concentration of a solute based on the molar absorptivity (ε) at the absorption maximum (λ_{max}). This process is aided by the use of the ***Beer–Lambert law*** (aka *Beer's law*) plot where the absorption (*Abs*) at the λ_{max} is plotted against the known concentration of a set of standards. An example Beer's law plot is shown below; this data was collected using a 1 cm path length cell.

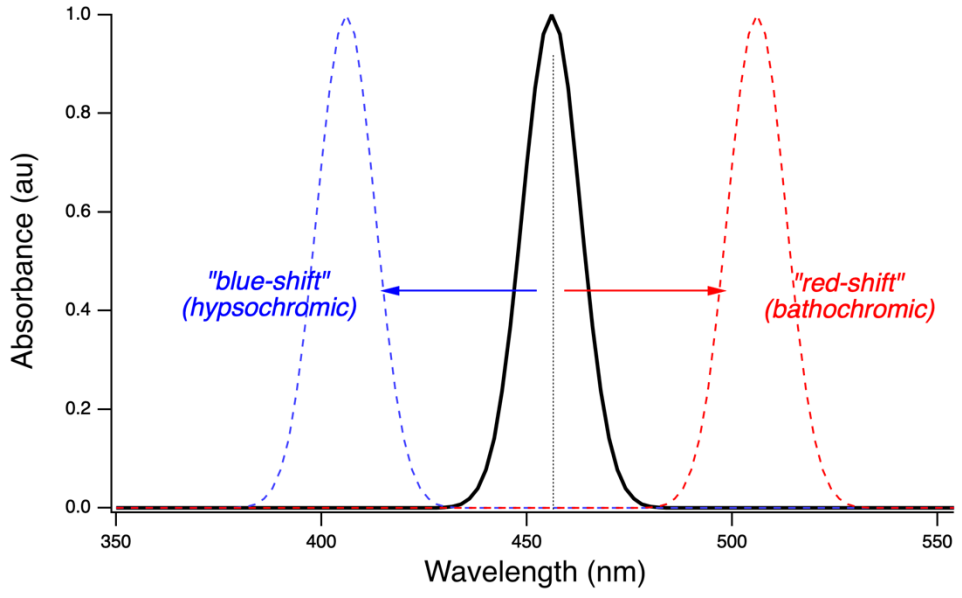


1a) Using the data above, if an unknown solution has an absorbance measurement of 0.553, what is the concentration of this sample. Please answer this question using the *fit-line equation* to determine a precise answer.

1b) From the data above, what is the numerical value for the *molar absorptivity coefficient* (ε) for the solute under investigation?

1c) Can you explain why the concentration of the standards are 1x, 2x, 4x, 8x and not something like 1x, 2x, 3x, 4x?

2) This introductory UV-Vis spectroscopy discussion is followed in more advanced courses to include a conversation about ***red*** and ***blue*** shifts. As indicated below, a ***red-shift*** or a ***blue-shift*** is an indication that a "change" has occurred. This change can be associated with a change in solvent used to dissolve the solute or a comparison of derivatives (ex. adding a functional group to a solute). These terms, ***red-shift*** and ***blue-shift***, are descriptive terms but often do not have a molecular explanation.



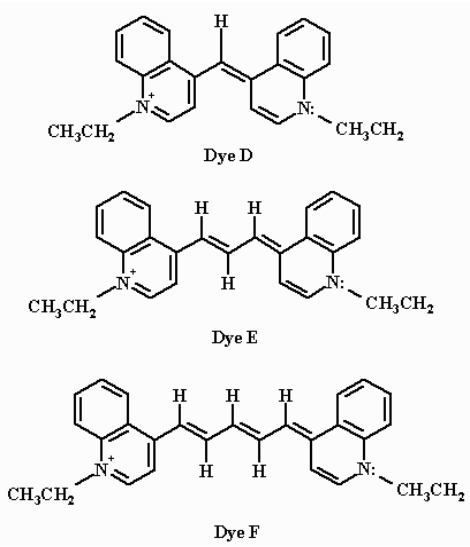
In quantum mechanics, the ***red-shift*** and ***blue-shift*** can be explained based on the particle in the box model. This model uses the fictious length (a) of a 1-dimensionl box to describe the "*molecular frame length*" for which the π-electrons exist. A change in the box length results in a change in the maximum absorbance wavelength (λ_{max}).

2a) If the UV-Vis spectrum of the dyes shown below were collected and overlaid in a single plot, the plot might look similar to the graph above. If this were the case, which dye is closest to the main absorbance (at 456 nm), which is closest to the ***red-shifted*** (506 nm) and which is closest to the ***blue-shifted*** (406 nm)…*focus only on the conjugated alkene moiety.*

Dye D → ***blue-shifted*** main ***red-shifted*** *(circle one)*

Dye E → ***blue-shifted*** main ***red-shifted*** *(circle one)*

Dye F → ***blue-shifted*** main ***red-shifted*** *(circle one)*



2c) Considering that a "single bond - double bond' arrangement is ~2.5 angstroms, this would make the above fictious box length of the dyes above to be ~2.5, 4.8, and 7.2 angstroms…again focusing only on *the conjugated alkene moiety…the bicyclic "end caps" can be considered the walls of the box.* Based on the estimated box lengths of 2.5, 4.8, and 7.2 angstroms calculate the λ_{max} for each of these compounds.

Please do these calculations one at a time and show all work!!!