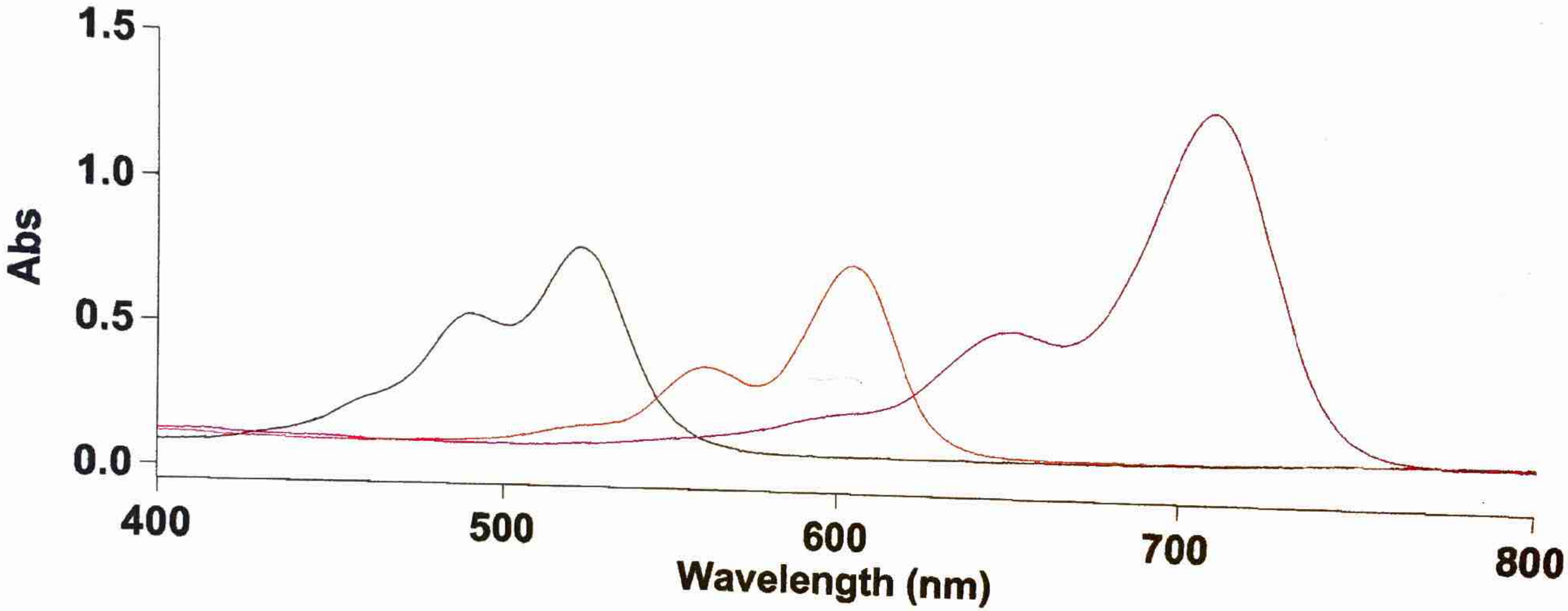
Sample Name: blue smaple 3

Collection Time	9/15/2016 3:32:03 PM
Peak Table	
Peak Style	Peaks
Peak Threshold	0.0100
Range	800.00nm to 399.73nm

Wavelength (nm)	Abs
603.53	0.752
560.24	0.387

TTU



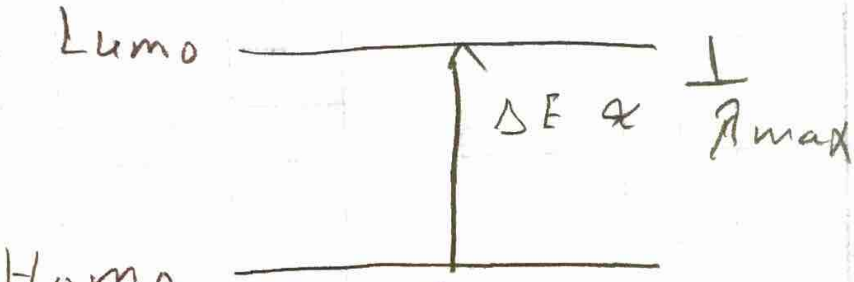
Scan Analysis Report

Report Time : Thu 15 Sep 03:26:10 PM 2016
Method:
Batch: C:\Documents and Settings\student\Desktop\pchem2.DSW
Software version: 3.00(339)
Operator:

Scan Analysis Report

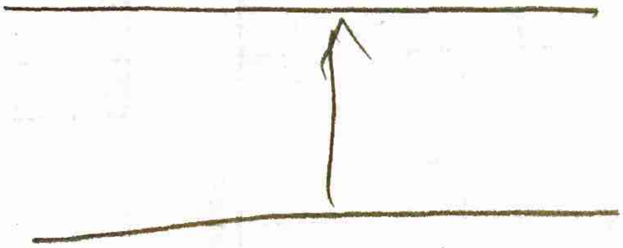
Report Time : Thu 15 Sep 03:29:19 PM 2016
Method:
Batch: C:\Documents and Settings\student\Desktop\pchem3.DSW
Software version: 3.00(339)
Operator:

Data	Shoulder nm	Side	λ_{max}
Pink	459.9	490.7	522.7
Blue	525.2	559.3	603.2
Light Blue	601.2	649.9	705.7



$\propto \frac{1}{L^2}$

Big Box



Small Box

$$\lambda = \frac{8mc\,(P+3)^2\,\ell^2}{h(P+3+1)}$$

$$\lambda = \frac{8mc\,\ell^2\,(P+3)^2}{h\,(P+4)}$$

$h = 6.626 \times 10^{-34}$ kg m²/s

$\ell = 1.39\,A^{\circ} = 0.139$ nm

$c = 3 \times 10^{8}$ m/s

$m = 9.11 \times 10^{-31}$ kg

$$\lambda = 63.7\,\frac{(P+3)^2}{P+4}\ \text{nm}$$

43 $E_n = \frac{h^2 n^2}{8 m L^2}$ $n = 1, 2, 3, 4, \ldots$

$n_1 = N/2$ $n_2 = (N/2+1)$

$E_n = \frac{h^2}{8mL} (n_2^2 - n_1^2) = \frac{h^2}{8mL^2} \left(\frac{N^2}{4} + N + 1 - \frac{N^2}{4} \right)$

$E_n = \frac{h^2}{8mL^2} (N+1)$

$\Delta E \neq \cancel{h\nu} = \frac{hc}{\lambda}$

$\lambda = \frac{hc}{E} = \frac{hc\,(8mc^2)}{h^2 (N+1)}$

$\lambda = \frac{(8mcL^2)}{h(N+1)}$

1- P = number of carbon atoms in a polymethine

2- $N = P + 3$

3- Kuhn assumed that l = length of the chain between nitrogen atoms + one bond distance on each side $\rightarrow$ $L = (P+3)\,l$

SIGNATURE	DATE	WITNESS/TA	DATE

Q2

Dye #1

$\lambda_{max_1} = 328 nm$

$$\frac{1}{\lambda_{max}} = \frac{1}{328 nm} * \frac{10^{+9} nm}{10^2 cm} = 30488 cm^{-1}$$

$$E_1 = \frac{hc}{\lambda_{max}} = \frac{(6.626 \times 10^{-34})(3 \times 10^8)}{328 \times 10^{-9}} \times \frac{6.022 \times 10^{23}}{1000 J/kJ}$$

$= 364.955 kJ/mol \approx 365 kJ/mol$

Dye #2

$$\frac{1}{\lambda_{max_2}} = 1/453 nm \times \frac{10^9 nm}{10^2 cm} = 22075 cm^{-1}$$

$$E_2 = \frac{hc}{\lambda_{max_2}} = \frac{(6.626 \times 10^{-34})(3 \times 18)}{453 \times 10^{-9}} \times \frac{6.022 \times 10^{23}}{1000 J/kJ}$$

$= 264.25 kJ/mol \approx 264 kJ/mol$

Dye #3

$$\frac{1}{\lambda_{max_3}} = 1/579 nm \times \frac{10^9 nm}{10^2 nm} = 17271 cm^{-1}$$

$$E_3 = \frac{hc}{\lambda_{max_3}} = \frac{(6.626 \times 10^{-3})(3 \times 10^8)}{579 \times 10^{-9}} \times \frac{6.022 \times 10^{23}}{1000 J/kJ}$$

$= 206.745 kJ/mol \approx 207 kJ/mol$

Q1 $\lambda_{max} = 63.7 \frac{(P+3)^2}{P+4}$ and P = number of carbon atoms in palymethine.

Dye #1 $P = 3$

$\lambda_{max} = 63.7 \frac{(P+3)^2}{P+4} = 63.7 \frac{(3+3)^2}{(3+4)} = 328 nm$

Dye # 2 $P = 5$

$\lambda_{max} = 63.7 \frac{(5+3)^2}{(5+4)} = 453 nm$

Dye #3 $P = 7$

$\lambda_{max} = 63.7 \frac{(7+3)^2}{(7+4)} = 579 nm$

For the Lab Report Calculation and Discussion

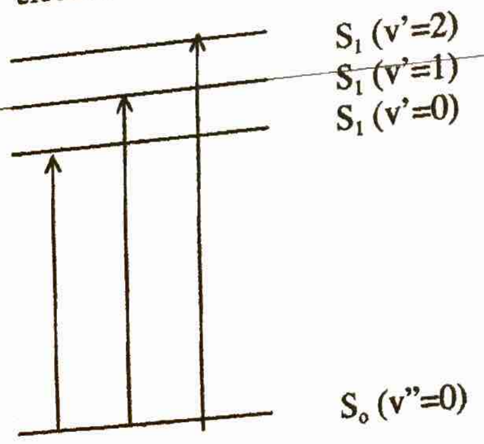
1. Calculate the purely theoretical λ_{max} in nm for each dye in the simplest particle-in-a-box model (the Kuhn Model) by using Equation (5) in the lab text ($\alpha = 0$); compare these values with your observed wavelengths.

2. Use Equation (6) to obtain the length adjustment factor α for each dye using their respective observed λ_{max} and the appropriate values of p. There is no need to calculate the uncertainty in α.

3. Take the mean value of α from #2 and use this single value $\langle\alpha\rangle$ to calculate λ_{max} for all these dyes; compare these to your observed values. Report your comparison for each dye as % absolute error on the lab report cover.

4. There is some ambiguity as to the values of P for the dyes, since the ring system allows extra space for the electrons to move. To investigate this repeat steps 1, 2, & 3 adding 1, 2, & 3 to all the values of P. Do this in a spreadsheet and deduce the best value for the contribution of the ring systems.

5. Notice that the spectrum for each dye shows a side peak and a shoulder to the high-energy side. These correspond to absorptions into excited vibrational levels of the electronically excited state. Shown schematically:



(Notation: In photochemistry, the lowest singlet state is S_o and the first excited singlet state is S_1. Also, v" and v' are the vibrational states in the ground and excited electronic states, respectively.)

Measure the positions of these side peaks (estimate the positions of the shoulders) and obtain the excited state vibrational frequencies (in cm^{-1}). [The vibrational frequency corresponds to the ***spacing*** between bands and ***not*** the absolute positions.] Sketch the spectrum and the corresponding energy level diagram, include the measured values (for one of the dyes) and label everything. From a table of organic IR group frequencies, identify the type of vibration that most closely matches the measured one. Is this appropriate to the dye molecule?

PHYSICAL CHEMISTRY LABORATORY

Experiment 34

Absorption Spectrum of a Conjugated Dye

Additional Reading: Garland et al, 8th ed., pp. 393-98, 618-36; Atkins & De Paula, pp. 288-92, problem 8.31, pp. 489-90, pp. 495–87, and p. 500 (section c).

Note: You can skip the error analysis in this experiment.

<u>Prelab for the Lab notebook:</u>

1. Calculate the purely theoretical λ_{max} in nm for each dye in the simplest particle-in-a-box model (the Kuhn Model) by using Equation (5) in the lab text ($\alpha = 0$).

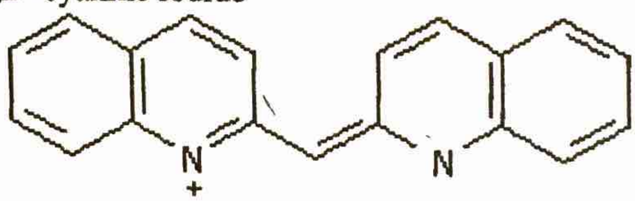
2. For the three wavelengths in question 1., calculate and tabulate the wavenumber (cm^{-1}) and excitation energy (kJ/mol) for each λ_{max}.

3. Derive Equation (5) and list various assumptions made in the Kuhn model. Include the calculation of the numerical factor 63.7 nm (show all work and units!).

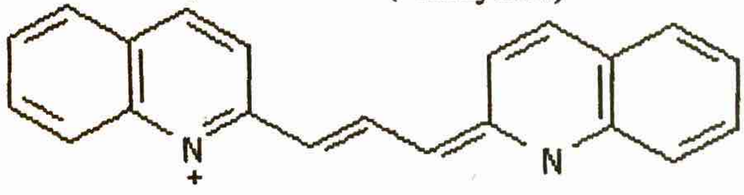
The Experiment

The experiment is described in the lab text; we will perform the experiment with the exception that the spectra will be obtained using the Perkin-Elmer Lambda 4B Spectrophotometer. The instructions for using this instrument are available in the P. Chem lab next to the instrument. The three dyes we will work with are (the ethyl groups are omitted):

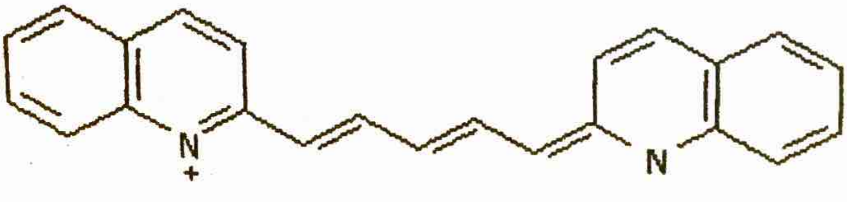
Dye 1: 1,1'-diethyl-2,2'-cyanine iodide



Dye 2: 1,1'-diethyl-2,2'-carbocyanine iodide (Pinacyanol)



Dye 3: 1,1'-diethyl-2,2'-dicarbocyanine iodide



Lab Report Checklist

_____1. Cover Sheet all filled in.

--Most fundamental result value reported
--Literature values referenced somewhere

_____2. Data and calculations.

--neatly tabulated
--sample calculation of every different type of calculation, **done by hand**
(one sample for every column of the spreadsheet)
--UNITS everywhere!!!
--graphs include Legend with slope, intercept, error bounds, etc.

_____3. Full table of results, both intermediate and final (final results go on cover page)

_____4. Discussion

--does the error bound include the accepted value?
--dominant source of error
--discussion questions from handout or lab text

_____5. Attached spectra or other chart recorder traces (photocopies are ok)

_____6. Recall format for reporting values with uncertainties:

--Round **uncertainties** to <u>two</u> significant digits.
--Round **values** consistent with their uncertainties.
--Examples:

$$17.46271 \pm 0.01186 \text{ mol L}^{-1} \quad \textit{becomes} \quad 17.463 \pm 0.012 \text{ mol L}^{-1}$$

↑ ↑ ↑ ↑

Note the format in scientific notation:

$$(2.974 \pm 0.014) \times 10^{-8} \text{ m}^2/\text{s}$$

↑ ↑

rev. F2015

PHYSICAL CHEMISTRY LAB REPORT

NAME:
Group #:

DATE LAB WORK COMPLETED:

DATE HANDED IN:

LAB Section:
Tues. 3-6___ Tues. 6-9___ Wed. 3-6___ Wed. 6-9___ Thurs. 3-6___ Thurs. 6-9___

Experiment # and Title:

Grade =

Lab notebook (15%) =

Calculations (20%) =

Error analysis (25%) =

Discussion (25%) =

Results (15%) =

Lateness (3 pts/day)

I am presenting my original work for evaluation and have completed the *checklist on the reverse*.
Sign Here:____________________

Results:

Experimental

Theoretical
or Literature values (source)

Percent relative error

Percent absolute error

Outline of a Lab Report (these are the appropriate section headings)

Cover Sheet - available in lab.

Experimental Procedure - briefly indicate *deviations* from the procedure in the manual or handout.

Purpose: Describe the most fundamental quantity that is measured in the experiment.

Primary Data - neatly labeled tables of the data taken in the laboratory.

Sample Calculations – A sample one of each kind of calculation done in the report, starting with the primary data and working toward the necessary derived quantities. This should not simply be gobs of equations, but include a bit of prose between each equation explaining what is being done. ***These should be done by hand.*** (See p. 25 of Garland.)

Results - appropriate tables of derived quantities and recorder charts.

Error Analysis - include representative calculations demonstrating the propagation of uncertainties.

Discussion - describe any deviations from theoretical or accepted values.

Define the major source of error. (Which measurement introduced the major source of error?)

Answer question posed by the lab text or handout.

Appendix - any lengthy spreadsheets.

Lab reports should also generally look like the example in the lab text, pp. 10-25.

Since several students may be performing the experiment at the same time, there may be a temptation to copy. Students must ***present their own work*** for evaluation. Although students are free to discuss the experiments, lab reports that are too nearly the same as any other--INCLUDING REPORTS OF PAST YEARS, WHICH I HAVE ON FILE--will automatically be marked F for plagiarism (zero points).

Grading

The main criteria for assigning grades to a report will be how well the report communicates the results, quantifies the uncertainties, describes their derivation, and demonstrates comprehension of the experiment. **Due dates:** Lab reports will be due two weeks after the experiment is performed. Late reports will be penalized *3 points for every weekday* (the weekend counts as one day). After all the reports have been turned in for a given experiment, the whole set of reports will be graded together and handed back to the student. Once the reports are handed back to the class, no further late reports will be accepted for that experiment.

Lab Manual: *Garland, Nibler, and Shoemaker,* **Eighth edition**

General reading on the lab and reports:

pp. **1-28 (emphasize)**, 29-90 (important), 687-708, *719-720 (essential).*

This laboratory supplements the material covered in lecture. The lab grade is a portion of the final course grade corresponding to one credit. Students will perform the labs according to the schedule of experiments handout. Each individual student will keep their own data in their lab notebook and write their own lab reports.

The handout for each experiment contains the reading assignments of important background material. This is NOT suggested reading. The philosophy behind this modest amount of background reading is that each student should have a feeling for the experimental method and the equipment used in the experiment. The assigned material in the lab text, handouts, and other sources should be read before coming into the lab. *Preparedness* will help the student be more confident with the experiment and work more efficiently.

The bound lab notebook sold in the bookstore is required; bring one to the first lab period. All data taken in the lab should be entered directly into this. Recording data in a lab notebook is an important practice in documentation that will follow you throughout your professional career, perhaps even into a courtroom (if your are not careful). Before coming to lab you will also enter into your notebook the prelab calculations and questions from the lab handouts. The notebook pages will be signed, dated, and the carbon copies will be handed in before leaving lab.

Two other ideas will help make the lab a better learning experience. After an experimental setup has been assembled and before starting the procedure, have the instructor check the setup and ask the instructor to describe any points of misunderstanding or confusion. Before leaving the lab the student should make a mental rundown of the calculations to be performed to be certain of having all the data needed. This includes the very important errors estimated for the measurements made.

<u>Lab Reports</u>

A written lab report will be handed in by each student for each experiment. There are two objectives of the lab reports of approximately equal value. The reports should be written from the perspective of communicating to any interested outside observer the important details of the experiment, as if the experiment had never been done before and the results are new. The reports also should be prepared to demonstrate to the instructor a comprehension of the principles of the experiment, the associated analysis of the data and uncertainties, and an interpretation of the results. Preparation of lab reports should be carried out with these two objectives in mind. Lab reports should be neat, but typing is not necessary.