Analyzing the Kinetics of a Bromophenol Blue Fading Reaction in Basic Conditions for an Undergraduate Lab

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1.

Background

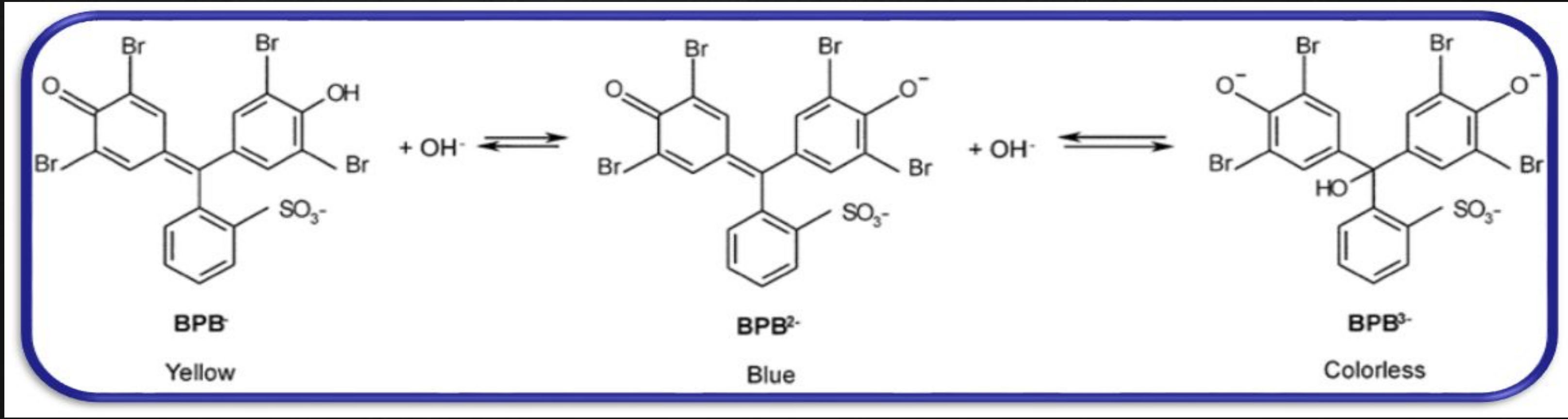
Chemical Kinetics and Spectrometry

- Kinetics labs can be performed in a wide variety of undergraduate laboratory classes making research in the field important for chemical education
- History[1,2]:
  - **1814**: Fraunhofer invents the spectroscope in Bavaria–known as the Father of the Spectrometer
  - **1850**: Wilhelmy found that the rate of inversion of sucrose is directly proportional to the concentrations of the reactants, sugar and acid
  - **1859**: Bunsen and Kirchhoff invent a spectroscope to use in the field of chemistry
  - **1864**: Guldberg and Waage proposed that the reaction "forces" are proportional to the product of the concentrations of the reactants: $K = [R]^r [S]^s / ([A]^a [B]^b)$
  - **1865**: Harcourt and Esson determined the concentration vs. time relationships of a kinetics experiment and integrated corresponding differential equations
  - **1884**: van't Hoff published "Studies of Chemical Dynamics"
  - **1887**: Ostwald coins the terms "reaction order" and "half-life"

- Chemical kinetics is used to study the speed at which a chemical or physical reaction occurs[3]
- By performing kinetics experiments, students can determine rate laws, rate constants and orders of reaction
- For this laboratory write-up, the main focus is on the use of absorbance versus time data, half-lives and calculating rate constants to determine the reaction order as well as the order in respect to the two reactants, bromophenol blue and NaOH
- In order to do so, a solution consisting of mainly concentrated base and a small amount of dye solution is used

Bromophenol Blue v. NaOH[5]

- The reaction with bromophenol blue in a concentrated basic solution, NaOH, is a pseudo-first order reaction according to literature research[6]
- This means when that while the reaction is a second order kinetics reaction, when the base is present in great excess compared to the dye, the reaction acts as a first-order reaction with respect to the reactants



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Method

Materials

- USB4000 Ocean Optics Spectrometer
- OceanView Software
- $3.73*10^{-4}$ M solution of Bromophenol Blue
- 4M and 2M solutions of NaOH
- Pipettes
- Cuvettes
- Parafilm

Using the Ocean Optics Spectrometer to Run Experiment

- The Ocean Optics spectrometer is paired with OceanView software that collects data in real time
- First, an absorbance spectrum was obtained for bromophenol blue to determine the optimal wavelength
- Using the determined wavelength, the stripchart option in OceanView was used to run the kinetics experiment

How the Ocean Optics Spectrometer Works

Light Source → Sample → Spectrometer → Computer

- A source of radiation comes from an attachment and travels through the sample cell into the spectrometer
- A collimating mirror reflects the incoming radiation onto the diffraction grating
- Diffraction grating separates the wavelengths of light onto the focusing mirror
- Focusing mirror reflects the wavelengths of light onto the diode array detector
- Diode array detector detects/records the varying wavelengths and through a USB connection, the data is collected in the OceanView software

Rate Law Calculations

Solution A: Bromophenol blue and 4M NaOH
Solution B: Bromophenol blue and 2M NaOH

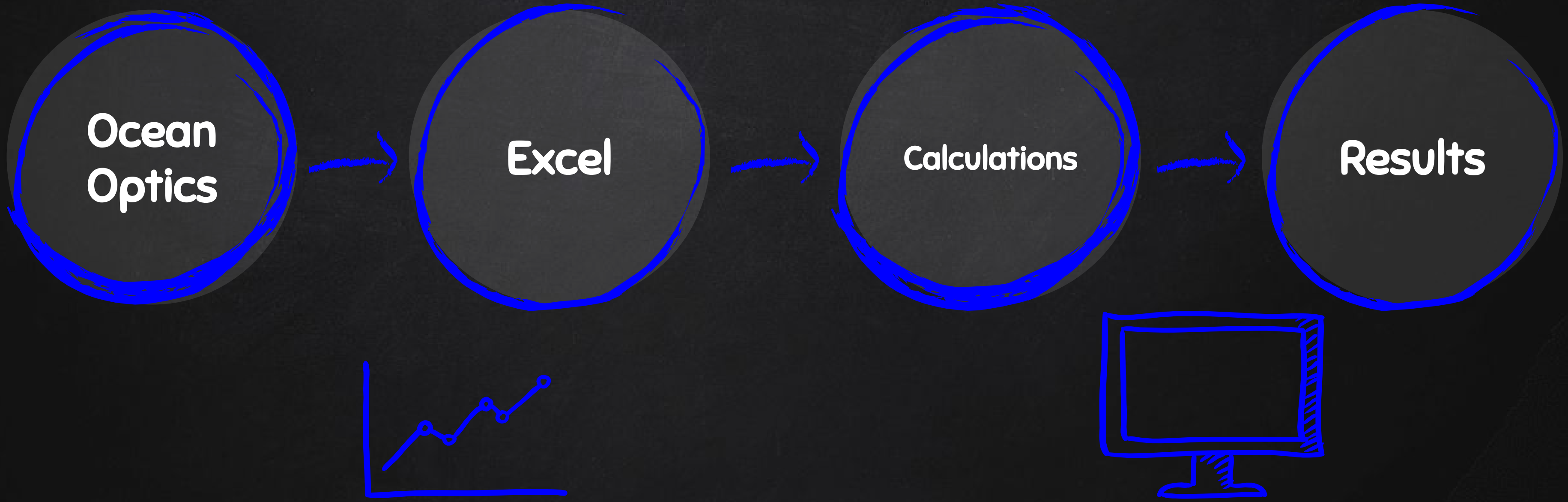
$t_{\frac{1}{2}}(A)$ → $$k(A) = \frac{\ln(2)}{t_{\frac{1}{2}}(A)}$$ → $k(A)$

$t_{\frac{1}{2}}(B)$ → $$k(B) = \frac{\ln(2)}{t_{\frac{1}{2}}(B)}$$ → $k(B)$

$$n = \frac{\ln\left[\frac{k(A)}{k(B)}\right]}{\ln\left[\frac{Molarity\ (A)}{Molarity\ (B)}\right]}$$

$n =$ *order with respect to the* OH^- *concentration*

Experimental Scheme



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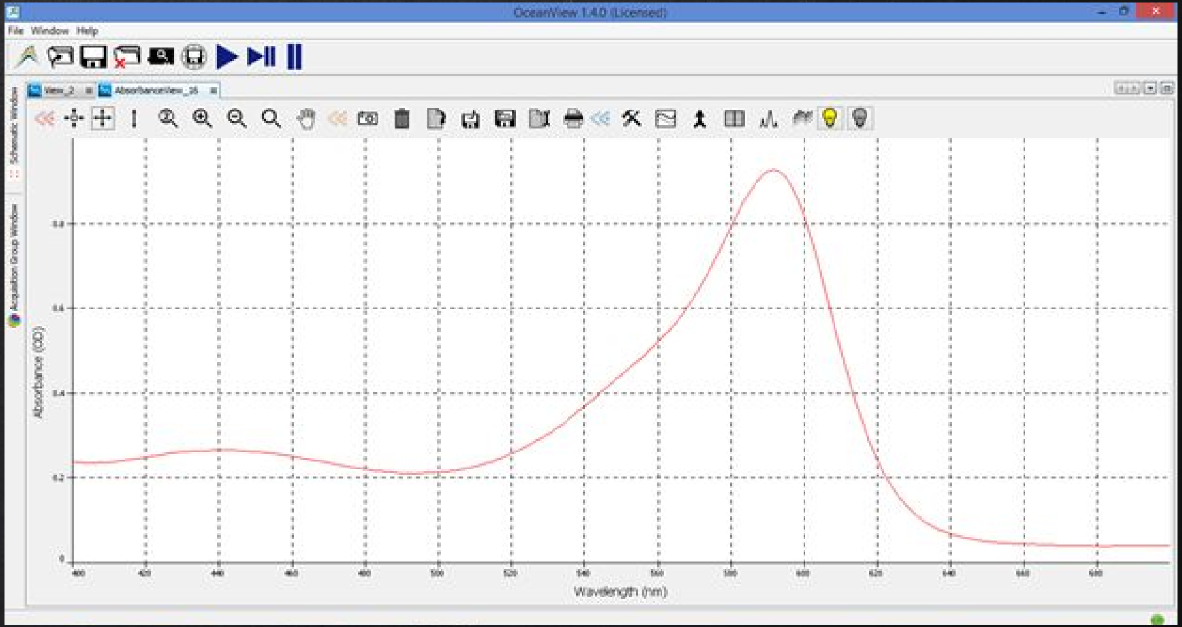
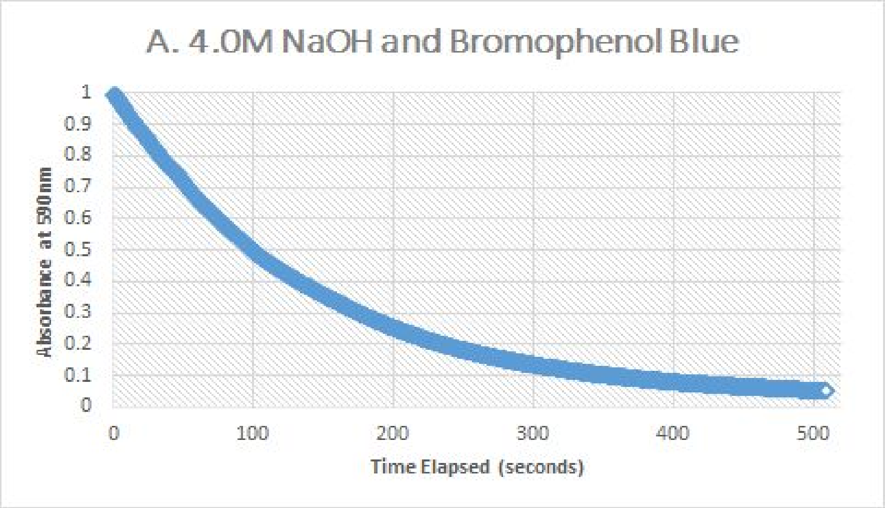
Results

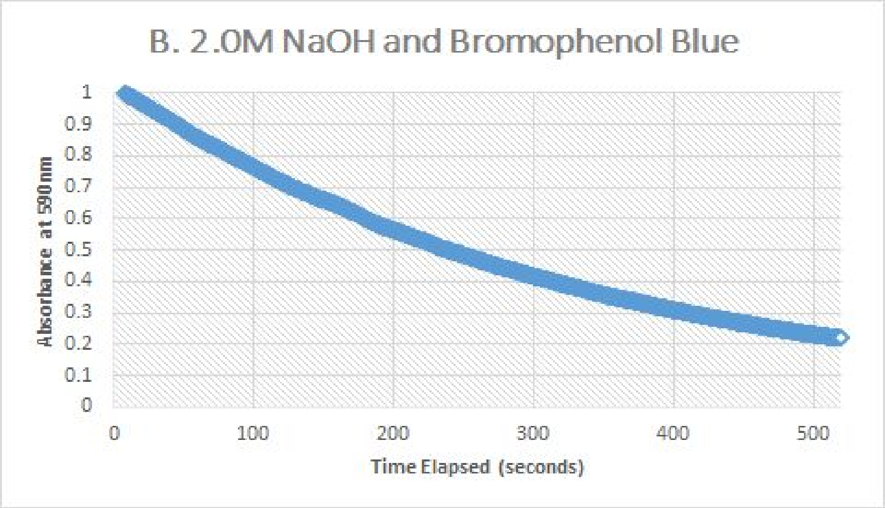
Determining the Appropriate Wavelength for Bromophenol Blue



From the absorbance spectrum of bromophenol blue, it can be seen that the wavelength at 590nm is the best to use in this experiment which is also supported by literature research[7]

Absorbance Vs. Time





Once the raw data from Ocean Optics is exported to Microsoft Excel, the real time data can be converted to form Absorbance v. Time graphs

Half-Life Calculation for Reaction A

Absorbance	Time (seconds)	Half-Life (seconds)
1.001	0.000	
0.501	99.140	
		99.140
0.997	3.340	
0.499	99.790	
		96.450
0.871	20.960	
0.434	119.850	
		98.890
0.778	37.940	
0.389	136.820	
		98.880
0.620	69.780	
0.301	174.770	
		104.990

Average Experimental Half-Life for Reaction A:

99.491 seconds

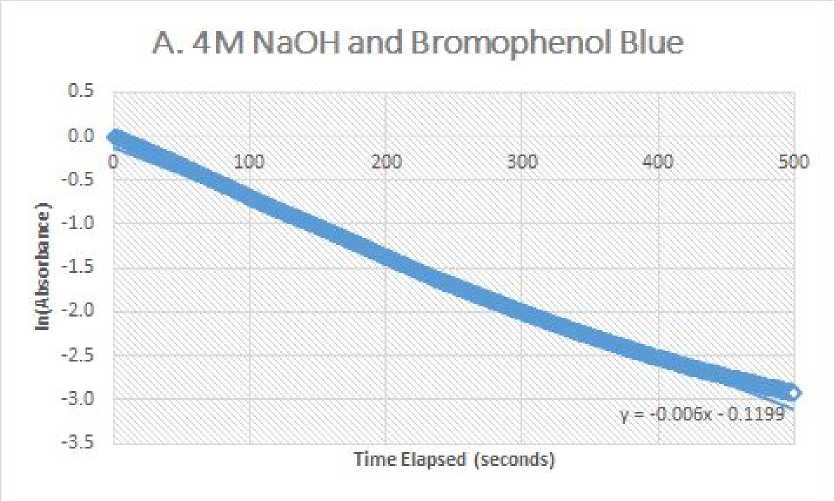
Half-Life Calculation for Reaction B

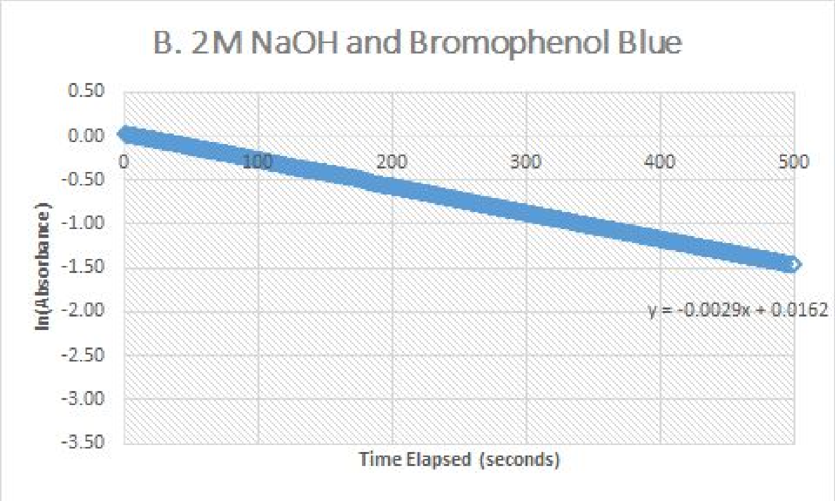
Absorbance	Time (seconds)	Half-Life (seconds)
1.002	7.470	
0.500	238.380	
		230.920
0.987	13.430	
0.493	243.100	
		229.670
0.864	57.460	
0.4310	288.050	
		230.590
0.683	136.360	
0.342	366.810	
		230.460
0.571	200.250	
0.281	432.150	
		231.900

Average Experimental Half-Life for Reaction B:

230.710 seconds

Order with Respect to Bromophenol Blue





- In order to determine the order of reaction with respect to Bromophenol Blue, the data was graphed ln(Absorbance)/time
- Because they are both linear, the experimental data shows that the reaction is a first order reaction in respect to the indicator

Order with Respect to NaOH

- $t_{1/2}$(A)= 99.491 seconds
  - $k(A) = \ln(2)/t_{1/2}(A)$
    - k(A)= 0.007

- $t_{1/2}$(B)= 230.710 seconds
  - $k(B) = \ln(2)/t_{1/2}(B)$
    - k(B)= 0.003

$$n = \frac{\ln[0.007/0.003]}{\ln[4M/2M]} = 1.19$$

n=1.19 –> 1st order with respect to the hydroxide ion concentration

Overall Order of Reaction

Rate Law:

Rate=k $[BPB^-]^n$ $[OH^-]^m$

Order in respect to bromophenol blue: n=1

Order in respect to the hydroxide ion: m=1

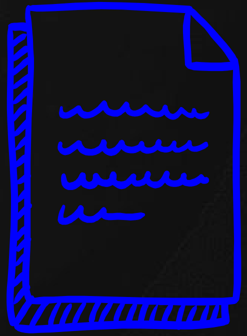
Overall order of reaction: 2

4.

Discussion

Discussion

- The experiment was successfully run using the Ocean Optics spectrometer
- The OceanView software allowed for the absorbance vs. time data to be collected
- Using Microsoft Excel, the necessary calculations were able to be done to calculate the rate orders
- In the end, it was determined that the experimental rate orders matched that of the literature research
- From all of this, accurate and helpful procedures were able to be written-up and provided for lab classes



Issues with Ocean Optics

- Throughout the entirety of the research performed, several problems arose while using the Ocean Optics spectrometer:
  - The OceanView software gives data in real time, meaning a somewhat time consuming process of converting time in excel is necessary
  - The OceanView software can also only collect/store a limited number of data points, so reactions must occur in a certain time frame

Converting time to decimal

Time from Ocean Optics	Time Hours	Hours Decimal	Minutes Decimal	Seconds Decimal	Seconds Difference	Seconds Cummulative
47:47.0	9:47:47 AM	9.796389	587.783	35267.000	0.000	
47:48.2	9:47:48 AM	9.796719	587.803	35268.189	1.189	0
47:49.1	9:47:49 AM	9.796962	587.818	35269.064	0.875	0.875
47:49.9	9:47:50 AM	9.797201	587.832	35269.924	0.860	1.735
47:50.8	9:47:51 AM	9.797448	587.847	35270.814	0.890	2.625
47:51.7	9:47:52 AM	9.797687	587.861	35271.674	0.860	3.485
47:52.5	9:47:53 AM	9.797930	587.876	35272.549	0.875	4.360
47:53.4	9:47:53 AM	9.798169	587.890	35273.408	0.859	5.219
47:54.3	9:47:54 AM	9.798412	587.905	35274.283	0.875	6.094
47:55.2	9:47:55 AM	9.798655	587.919	35275.158	0.875	6.969
47:56.0	9:47:56 AM	9.798894	587.934	35276.017	0.859	7.828

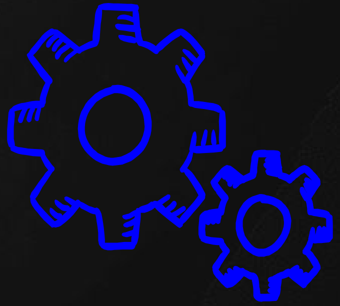
A5	Time from Ocean Optics data file
B5	Change format to hours:min:sec
C5 =	(B5-INTB5))*24
D5=	C5*60
E5=	D5*60
F6=	E6-E5
G7=	F7+G6

Now absorbance can be plotted against seconds cummulative.

5.

Conclusion

- Using the Ocean Optics spectrometer allowed for the rate order to be determined in respect to bromophenol blue, NaOH, and the overall reaction
- When compared to literature, the experimental results matched
- Because the experiment was deemed successful, the written up procedures and step-by-step instrumental instructions can be used in various lab classes as well as further research in kinetics experiments



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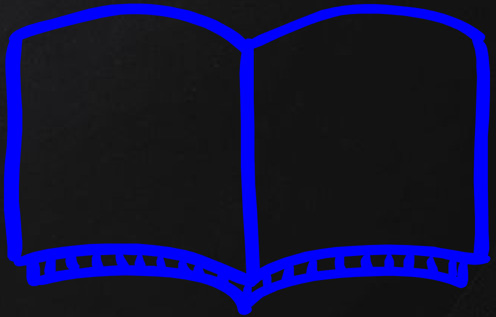
Future Work

Continuing Research

- I will be writing up a experimental procedure for the Fading of Bromophenol Blue and NaOH using the Ocean Optics spectrometer



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8.

References

[1]Espenson, J.H. *Chemical Kinetics and Reaction Mechanisms.* McGraw-Hill. 2nd ed. (**2002**). p.254-256.
[2]Hoff, J. H. van't (Jacobus Henricus van't); Cohen, Ernst; Ewan, Thomas. *Studies in chemical dynamics.* Amsterdam : F. Muller ; London : Williams & Norgate. (**1896**).
[3]Steinfeld J.I., Francisco J.S. and Hase W.L. *Chemical Kinetics and Dynamics.* Prentice-Hall. (**1999**) p.94-97.
[4]Santa Cruz Biotechnology, Inc. Bromophenol Blue (CAS 115-39-9) Properties.
[5]Winans, Randall; Brown, Charles A. Fading of bromophenol blue. A combined synthesis and spectrophotometric kinetics experiment. *Journal of Chemical Education.* (**1975**) *52* (8), 526.
[6]Fieser, L. F., and Fieser, M., "Topics in Organic Chemistry," Reinhold Publishing Corp., New York, **1963**, p. 368-71
[7]Kolthoff, I. M., "Acid-Base Indicators," (Translator: Rosenblum, C.) MacMillan Co., New York, 1937.
[8]Lalanne, R., J. CHEM. EDUC., **48**, 266 (1971).
[9]Adams, R., Johnson, J. R., and Wilcox, C. F., "Laboratory Experiments in Organic Chemistry," 6th Ed., MacMillan Co., New York, **1970**, p. 426-9.
[10]Amis, E. S., and LaMer, V. K., *J. Amer. Chem. Soc.*, **61**, 905 (1939); Sager, E. E., Margatt, A. A., and Schooley, M. R., *J. Amer. Chem. Soc.*, **70**, 732 (1948).
[11]Freas, R., and Provine, E. A., *J. Amer. Chem. Soc.*, **70**, 732 (1948).
[12]Wiberg, K. B., "Computer Programming for Chemists," W. A. Benjamin, Inc., New York, **1965**, p. 41.

Questions?