Organic Chemistry 211 Laboratory
Nucleophilic Substitution of Alkyl Halides

(Part 3: Effect of Change in Temperature on the S_N1 Reaction Rates)

Waste Disposal: All the reaction mixtures should be placed in the halogenated organic waste container.

Objective: To study the effects of changing the reaction temperature on the rate of S_N1 reactions.

Experiment Overview: One of the reactions of part 2 will be studied, at 5 different temperatures; (10, 20, 30, 40, 50)^{o}C. The temperature will be the only variable, all else being constant.

Procedure:

From your results in part 2, select the solvent system for which the neutralization time at 30°C is close to 10 minutes. Place five 2 mL portions of this solvent in test tubes, to each test tube add 3 drops of phenolphthalein. Set up the water bath apparatus as you did in part 2. It is easier to start with the high temperature (50°C) and work towards the lower temperatures.
Similar to part 2 of this experiment, record the time it takes for the pink, basic, phenolphthalein to become colorless.
After having obtained the 5 data points, <u>manually</u> plot a *log t (t = reaction time in seconds)* versus 1/T (T = temperature, in Kelvins), draw a best fit straight line, and calculate the slope for the line. Using the value for the slope, you could calculate the activation energy for the reaction. According to the equation (1) shown below, the rate constant is a function of the temperature of a reaction. Plotting the graph based on the equation (1) will result in an exponential curve, whereas the logarithmic form of this equation, (i.e., equation 2) will yield a straight line:

$$k = A \exp\left(-\frac{E_a}{RT}\right) \qquad \textbf{Eq. 1}$$

$$\log k = \log A - \frac{E_a}{2.3R}\left(\frac{1}{T}\right) \qquad \textbf{Eq. 2}$$

Note: The straight line you draw will serve as a *reference line*, therefore you should choose two points from the line (not your data points) to calculate the slope. This is a general routine in the usage of the reference curves and lines.

For your report:
Draw the graph.
Discuss the general trend for the change in the reaction rate as a result of change in the temperature.

Needed per student:

solvent systems (same as in part 2)

t- butyl chloride (0.5 mL)---------------------------------→ 8 mL per laboratory

Styrofoam cups (1)---------------------------------------→ 15 per laboratory

NaOH (0.5 M) --→ 2 small dropper bottles per lab

Phenolphthalein indicator--------------------------------→ 2 dropper bottles per laboratory

Timer (1)---→ 15 per laboratory