During Class Invention

Temperature Dependence of the Rate Constant

Name___________________________

TA Name ______________________

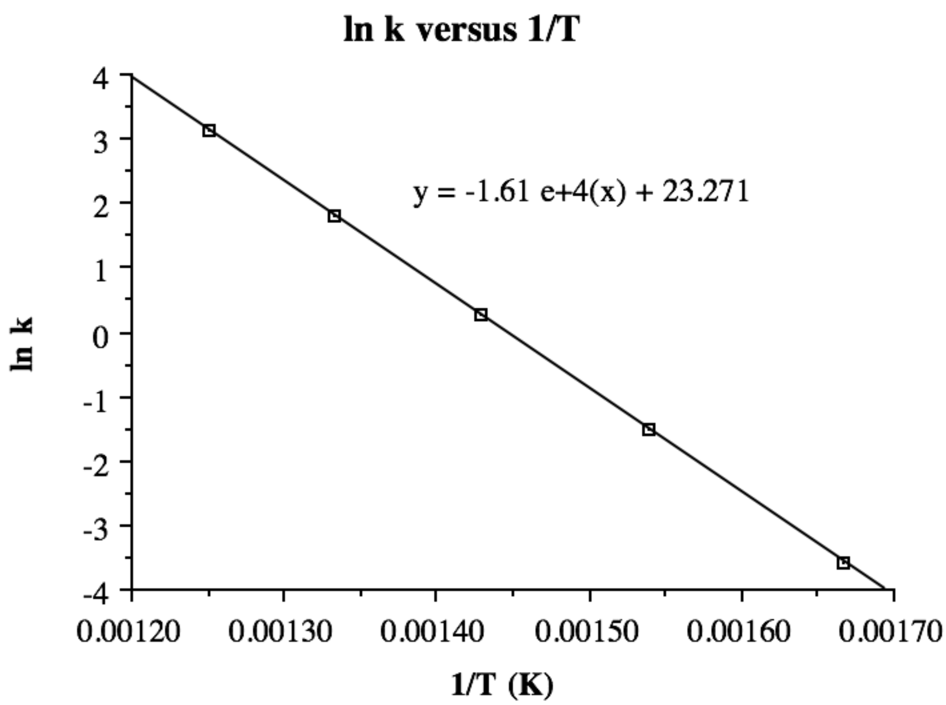
Lab Section #______

1a. The following rate data was obtained at different temperatures for the reaction

$$O_3(g) + NO(g) \rightarrow O_2(g) + NO_2(g)$$

Temperature (K)	k ($M^{-1}\cdot sec^{-1}$)
600	0.28
650	0.22
700	1.30
750	6.00
800	23.0

Sketch the plot of *ln* k (*y*-axis) versus $\frac{1}{\text{temperature}}$ (*x*-axis) .



b. Write the Arrhenius equation and identify each term

$$\ln\left(\frac{k_1}{k_2}\right) = \frac{E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

k_1 and k_2 are both rate constants at T_1 and T_2, respectively. E_a is the activation energy for the reaction and R is the ideal gas constant. The value of R is 8.314 $\frac{J}{mol{\cdot}K}$.

c. Define the term *activation energy*.

The activation energy, E_a, represents a measure of the energy barrier colliding molecules must surmount if they are to react rather than to recoil from one another. It is assumed that every pair of molecules with energy less than E_a will not react and every pair with energy greater than E_a and the proper orientation will react.

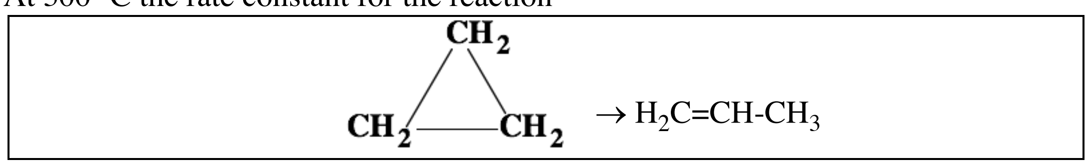
d. Determine the activation energy in the plot y ou made at the beginning of this problem.

From the plot

$$\text{Slope} = -1.61 \times 10^4 = -\frac{E_a}{R}$$

$$E_a = 1.61 \times 10^4\ \text{K} \cdot 8.314\ \frac{J}{mol{\cdot}K} = 134\ \frac{kJ}{mol}$$

2a. At 300 ˚C the rate constant for the reaction



is 2.41 x 10^{-10} sec^{-1}. At 400 ˚C the rate constant is 1.16 x 10^{-6} sec^{-1}. Calculate the activation energy for the reaction.

$$\ln\left(\frac{1.16 \times 10^{-6}}{2.41 \times 10^{-10}}\right) = \frac{E_a}{R}\left(\frac{1}{573} - \frac{1}{673}\right)$$

$$8.479 = \frac{E_a}{8.314\ \frac{J}{mol{\cdot}K}}(2.593 \times 10^{-4})$$

$$E_a = 272\ \frac{kJ}{mol}$$

b. Estimate the rate of the rearrangement reaction at 800 ˚C.

$$\ln\left(\frac{k_1}{k_2}\right) = \frac{E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$\ln\left(\frac{1.16 \text{ x } 10^{-6}}{k_2}\right) = \frac{272000 \frac{J}{mol}}{8.314 \frac{J}{mol \cdot K}}\left(\frac{1}{1073 \text{ K}} - \frac{1}{673 \text{ K}}\right)$$

$$\ln\left(\frac{1.16 \text{ x } 10^{-6}}{k_2}\right) = 32716 \text{ K } (-5.54 \text{ x } 10^{-4} \text{ K}^{-1})$$

$$\ln\left(\frac{1.16 \text{ x } 10^{-6}}{k_2}\right) = -18.1$$

take the exp() of both sides

$$\exp(\ln\left(\frac{1.16 \text{ x } 10^{-6}}{k_2}\right)) = e^{-18.1}$$

$$\frac{1.16 \text{ x } 10^{-6}}{k_2} = 1.38 \text{ x } 10^{-8}$$

$$k_2 = 84.1 \text{ s}^{-1}$$

c. If the activation energy for the decomposition of N_2O_5 is 1.0 x $10^2 \frac{kJ}{mol}$, calculate the temperature change necessary to double the rate at room temperature.

The rate constant, k_2, at the higher temperature will twice the rate constant, k_1, at the lower temperature. This can be expressed as,

$$k_2 = 2k_1$$

and substituted in the Arrhenius equation. The problem specifies E_a, and that the T_1 can be assumed to be room temperature, or 298 K. Given the Arrhenius equation,

$$\ln\left(\frac{k_1}{k_2}\right) = \frac{E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

and substituting,

$$\ln\left(\frac{k_1}{2k_1}\right) = \frac{100000 \frac{J}{mol}}{8.314 \frac{J}{mol \cdot K}}\left(\frac{1}{T_2} - \frac{1}{298}\right)$$

$$\ln\left(\frac{1}{2}\right) = 1.20 \text{ x } 10^4 \text{ K}\left(\frac{1}{T_2} - 3.36 \text{ x } 10^{-3} \text{ K}^{-1}\right)$$

$$-0.693 = 1.20 \text{ x } 10^4 \text{ K}\left(\frac{1}{T_2} - 3.36 \text{ x } 10^{-3} \text{ K}^{-1}\right)$$

$$-5.78 \text{ x } 10^{-5} \text{ K}^{-1} = \left(\frac{1}{T_2} - 3.36 \text{ x } 10^{-3} \text{ K}^{-1}\right)$$

$$\frac{1}{T_2} = 3.30 \text{ x } 10^{-3} \text{ K}^{-1} \qquad T_2 = 303 \text{ K} \text{ Therefore, } \Delta T = 5 \text{ K}$$

3. Sketch the energy profile diagram for the exothermic reaction

$$NO(g) + O_3(g) \rightarrow NO_2(g) + O_2(g)$$

and label the important features, including reactants, products, activated complex, the energy of activation and the enthalpy of the reaction. **See Appendix III for recommended demonstration, video, or computer resources.**