CH302H – Principles of Chemistry II: Honors
Fall 2016, Unique 49420

Homework, Week 14
(It is very likely we won't get through all of the material needed for this HW this week. Please come back to any questions you don't understand next week.)

1. What are the units of the pre-exponential factor A in the Arrhenius equation?

2. Initial rates for the following reaction have been obtained at a variety of temperatures:

$$OH(g) + ClCH_2CH_2Cl(g) \rightarrow H_2O(g) + ClCHCH_2Cl(g)$$

T (K)	k (10^8 L mol^{-1} s^{-1})
292	1.24
296	1.32
321	1.81
333	2.08
343	2.29
363	2.75

a) Determine the values of E_a and A for this reaction.

b) At what temperature will the rate of the reaction be twice the rate measured at 363 K?

3. Cyclohexane converts between two stable structures, the so-called "chair" and "boat" conformations. The enthalpy and entropy of the formation of the activated complex are known to be 31.9 KJ mol^{-1} and 16.7 J K^{-1} mol^{-1}, respectively.

a) Determine the Gibbs energy of activation and the rate constant for this conversion.

b) Based on the value of the enthalpy and entropy of the activated complex, hypothesize what the structure of the transition state might be.

4. $H_2(g)$ and $I_2(g)$ react in one elementary step to form HI.

a) Write out this reaction mechanism.

b) The entropy of the transition state is known to be > 0. Use all of this information to propose a structure of the transition state.

5. The reaction $H(g) + H_2(g) \rightarrow H_2(g) + H(g)$ has been studied extensively to understand basic mechanisms of gas phase reaction dynamics. A contour plot of the potential energy surface of the collinear collision of H and H_2 is shown below, where r_{12} is the bond length of the reactant H_2 and r_{23} is the bond length of the product H_2.

a) Label the transition state.

b) Draw a dashed line that indicates the lowest energy path of the reaction.

c) What is the distance between H and each hydrogen of the H_2 atom in the transition state? A drawing of the transition state would probably help you answer this problem succinctly.