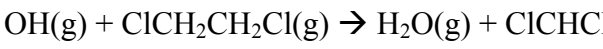
**CH353 – Physical Chemistry I**
Spring 2013, Unique 52575

**Homework, Week 15**

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

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.