

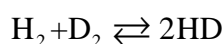
Seoul National University
Department of Materials Science and Engineering

Final Examination
 Physical Chemistry of Materials 2

December 17, 2012
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1. The hydrofluoric acid molecule (HF) has a moment of inertia of $1.34 \times 10^{-40} \text{ g} \cdot \text{cm}^2$. Calculate the rotational energy jump from the quantum state $J=0$ to the quantum state $J=1$. (10 pt)
2. The degeneracies of the singlet (paired electron spins) or triplet (unpaired spins) levels of a certain molecule are 1 and 3, respectively. The energy of the singlet state is greater than that of the triplet by a factor of ε .
 - (a) Write the electronic partition function of the molecule.
 - (b) Given that the factor $\varepsilon = 1.38 \times 10^{-14} \text{ erg}$ and $T=100 \text{ K}$, calculate the ratio of the population of the singlet level to the population of the triplet level. (10 pt)

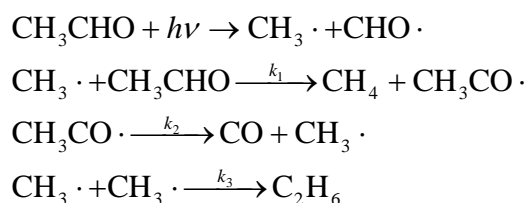
3. Calculate the equilibrium constant for the reaction at 300 K (15 pt)



using the following data:

| | H ₂ | HD | D ₂ |
|---|----------------|-------|----------------|
| Fundamental vibration $\nu \text{ (cm}^{-1}\text{)}$ | 4371 | 3785 | 3092 |
| Moment of inertia $I \text{ (g} \cdot \text{cm}^2 \times 10^{40}\text{)}$ | 0.458 | 0.613 | 0.919 |

4. The thermal conductivity of Ar at 300 K and 1 bar pressure is $0.0177 \text{ JK}^{-1}\text{m}^{-1}\text{s}^{-1}$. What is the collisional cross section of Ar assuming ideal gas behavior? (10 pt)
5. A certain reaction is first order, and at 540 s after initiation of the reaction, 32.5% of the reactant remains. (10 pt)
 - (a) What is the rate constant for this reaction?
 - (b) At what time after initiation of the reaction will 10% of the reactant remain?
6. The pre-exponential factor for the gas-phase decomposition of ozone at low pressures is $2.3 \times 10^{13} \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}$ and its activation energy is 30.0 kJ mol^{-1} . What are (a) the entropy of activation, (b) the enthalpy of activation and (c) the Gibbs energy of activation at 298 K?
7. A likely mechanism for the photolysis of acetaldehyde (10 pt)



Derive the rate law expression for the formation of CO based on this mechanism.

8. For a pair of electron donor and acceptor, $k_{et} = 2.02 \times 10^5 \text{ s}^{-1}$ for $\Delta G^\circ = -0.665 \text{ eV}$. The standard reaction Gibbs energy changes to $\Delta G^\circ = -0.975 \text{ eV}$ when a substituent is added to the electron acceptor and the rate constant for electron transfer changes to $k_{et} = 3.33 \times 10^6 \text{ s}^{-1}$. The experiments were conducted at 298 K . Assuming that the distance between donor and acceptor is the same in both experiments, estimate the values of the reorganization energy λ and the activation Gibbs energy ΔG^\ddagger . (15 pt)
9. The data below are for the chemisorption of hydrogen on copper powder at 25°C . Confirm that they fit the Langmuir isotherm at low coverages. Then find the value of K for the adsorption equilibrium and the adsorption volume corresponding to complete coverage. (10 pt)

| | | | | | | |
|-----------------|-------|-------|-------|-------|-------|-------|
| p/Pa | 25 | 129 | 253 | 540 | 1000 | 1593 |
| V/cm^3 | 0.042 | 0.163 | 0.221 | 0.321 | 0.411 | 0.471 |