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Department of Materials Science and Engineering

Final Examination December 17, 2012
Physical Chemistry of Materials 2 Professor Won Ho Jo

1. The hydrofluoric acid molecule (HF) has a moment of inertia of $1.34\times10^{-40}\ g\cdot cm^2$. 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 $\varepsilon = 1.38\times10^{-14}\ erg$ and *T*=100 *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)

   $$H_2 + D_2 \rightleftarrows 2HD$$

   using the following data:

	H_2	HD	D_2
Fundamental vibration $\nu\ (cm^{-1})$	4371	3785	3092
Moment of inertia $I\ \left(g\cdot cm^2\times10^{40}\right)$	0.458	0.613	0.919

4. The thermal conductivity of Ar at 300 *K* and 1 *bar* pressure is 0.0177 $JK^{-1}m^{-1}s^{-1}$. 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 $2.3\times10^{13}\ dm^3mol^{-1}s^{-1}$ 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)

   $$CH_3CHO + h\nu \rightarrow CH_3\cdot + CHO\cdot$$
   $$CH_3\cdot + CH_3CHO \xrightarrow{k_1} CH_4 + CH_3CO\cdot$$
   $$CH_3CO\cdot \xrightarrow{k_2} CO + CH_3\cdot$$
   $$CH_3\cdot + CH_3\cdot \xrightarrow{k_3} C_2H_6$$

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

8. For a pair of electron donor and acceptor, $k_{et} = 2.02 \times 10^5 s^{-1}$ for $\Delta G^\circ = -0.665 eV$. The standard reaction Gibbs energy changes to $\Delta G^\circ = -0.975 eV$ when a substituent is added to the electron acceptor and the rate constant for electron transfer changes to $k_{et} = 3.33 \times 10^6\ s^{-1}$. 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 $\Delta G^\ddagger$. (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