Discussion Section #10 – April 25, 2014

1. **Iodine Dissociation** Compute the dissociation constant K_p for iodine, $I_2 \rightarrow 2I$ at T=300K. The mass of an iodine atom is m_I=0.127kg/mol. The ground state electronic degeneracies of I and I_2 are 1 and 4 respectively. The rotational temperature and vibrational temperature of I_2 are 0.0537K and 308K respectively. The difference in the molar dissociation energy is -35.6kcal/mol.

2. In Homework #4, we learned that when molecues bind to a surface, some of their motions are transformed into different types of motion. That is, instead of translating like gas phase molecules in three dimensions, molecules in a surface adsorbed phase can translate only in two dimensions parallel to the surface, while their motion perpendicular to the surface has been transformed into a vibration of the "bond" holding the molecule to the surface.

Suppose one wall of cubic box with side length L=10cm is coated with a material that can bind helium atoms with a binding energy $E_{bind}=-\varepsilon$, where the magnitude of the binding energy per mole is N_A=100 kJ/mol. The other walls of the container do not bind helium. Thus, the surface vibrational state energies are $E_n=-\varepsilon+(n+1/2)h\nu_s$. For later, we will suppose that the magnitude o the ground state vibrational energy per mole of bound molecules is $N_A(h\nu_s/2)$=20kJ/mol.

a. As done in the homework, calculate the surface vibrational partition function of a helium atom.

b. Using your results from part (a), what is the partition function of a bound helium atom?

c. What is the partition function of an unbound helium atom?

d. Can you calculate the dissociation constant of *n* mole of helium atom from a metallic surface? If so, what is the dissociation constant K?

$$M(s) + nHe(g) \rightarrow nHe(g)$$