Fall 2008 CH301 Homework 13a Answer Key—Problems for Statistical Thermodynamics Lecture

1. Two quick ideas that make math with statistical thermodynamics a lot simpler:

a) What is the amount of energy for Avagadro's number multiplied by Boltzman's constant? What is the famous name of this value? kN = R = 8.314J the ideal gas law constant

b) Use what you know about log functions to simplify S=k lnW?

Let # = number of orientations in a molecule and let n = the number of molecules. $S=k \ln W = k \ln \#^n = n k \ln \#$

2. Answer the question asked about internal motional energy for each of the systems listed:

The number of degrees of freedom in a H atom in benzene? 3
The number of degrees of freedom in a benzene molecule? 36
The number of translational modes of motion in a molecule of benzene? 3
The number of rotational modes of motion in molecule of benzene? 3
The number of vibrational modes of motion in a molecule of benzene? 30
The number of degrees of freedom in 10 molecules of benzene? 360
The total internal motional energy in 10 molecules of benzene? 180kT
The total non-vibrational motional energy in 10 molecules of benzene? 30kT
The total vibrational energy in 10 molecules of benzene? 150kT
The total vibrational energy in a mole of benzene? 15RT
The total translational energy in 10 moles of benzene? 15RT
The number of degrees of freedom in 10 molecules of carbon monoxide? 60
The number of degrees of freedom in a O atom in carbon monoxide? 3
The number of translational modes of motion in a molecule of carbon monoxide? 3
The number of rotational modes of motion in molecule of carbon monoxide? 2
The number of vibrational modes of motion in a molecule of carbon monoxide? 1
The total internal motional energy in 10 molecules of carbon monoxide? 30kT
The total non-vibrational motional energy in 10 molecules of carbon monoxide? 25kT
The total vibrational energy in 10 molecules of carbon monoxide? 5kT
The total vibrational energy in a mole of carbon monoxide? 0.5RT
The total translational energy in 10 moles of carbon monoxide? 15RT

3. Which of the following molecules would have no positional entropy at absolute zero?

H_2 CH_4 NH_3 BH_3 SF_6 H_2O CO_2 COCl CH_3F I_3^- O_3

Answer: H_2 CH_4 BH_3 SF_6 CO_2 All the others can form more than a single crystal orientation.

4. Which of the following molecules would have a positional entropy closest to zero?

H_2O H_2S H_2Se

Answer: H_2O because it has the greatest IMF (due to H bonding.) The greater the IMF the more non-ideal the behavior and greater tendency to "order" thereby reducing the entropy.

5. Write an expression describing the maximum positional entropy of each of the following systems at absolute zero:

a) 1 molecule of ammonia $S = k \ln 4^1$
b) 10 molecules of carbon monoxide $S = 10\ k \ln 2$
c) a mole of chloromethane $S = k \ln 4N = kN \ln 4 = R \ln 4$
d) 50 molecules of BH_2Cl $S = 50\ k \ln 3$

e) 5 moles of CO_2 $S = 5R \ln 1 = 0$