CHE-371 Fall 2008

Homework #6

Chapter 20

1. Predict whether ΔS is positive or negative for the following reactions at 298K.
   i. $4\ Fe_{(s)} + 3O_{2(g)} \rightarrow 2\ Fe_2O_{3(s)}$
   ii. $O_{(g)} + O_{(g)} \rightarrow O_{2(g)}$
   iii. $NH_4Cl_{(s)} \rightarrow NH_{3(g)} + HCl_{(g)}$
   iv. $H_{2(g)} + Cl_{2(g)} \rightarrow 2HCl_{(g)}$

2. From the partition function for an ideal monatomic gas, you can express entropy:

$$\overline{S} = \frac{5}{2}R + R\ln\left[\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}\frac{\overline{V}g_{e1}}{N_A}\right]$$

   a. If you have 1 mole of He at 1 bar and 300 K in one container and 1 mole of Ar at 1 bar and 300 K in another, which will have a larger entropy?
   b. Consider (in thought) how the entropy expression would change for diatomic or polyatomic molecules. (Assume the major contributor to the entropy is the translational term.) Which molecule in the following pairs will have greater entropy under the same conditions?
      i. CO or CO_2
      ii. H_2O or D_2O
      iii. Methane or Ethane

3. Calculate the value of ΔS if one mole of an ideal gas is expanded reversibly and isothermally from 10.0 dm^3 to 20.0 dm^3. Explain the sign of ΔS.

4. Show that

$$\Delta S = C_p \ln\frac{T_2}{T_1}$$

   for a constant-pressure process if C_p is independent of temperature. Calculate the change in entropy of 2.00 moles of $H_2O(l)$ ($\overline{C}_p$ = 75.2 $J\cdot K^{-}1\cdot mol^{-1}$) if it is heated up from 10 °C to 90 °C.

5. Vaporization at the normal boiling point (T_{vap}) of a substance (the boiling point at 1 atm) can be regarded as a reversible processes. Calculate the entropy change when two moles of water vaporize at 100.0 °C. The value of $\Delta_{vap}\overline{H}$ is 40.65 $kJ\cdot mol^{-1}$. Comment on the sign of $\Delta_{vap}S$.

6. Calculate the entropy of mixing if two moles of N_2 (g) are mixed with one mole of O_2 (g) at the same temperature and pressure. Assume ideal behavior.

Chapter 21

1. The molar heat capacity of C2H4 (g) can be expressed by:

$$\overline{C}_V(T)/R = 16.4105 - \frac{6085.929\text{K}}{T} + \frac{822826\text{K}^2}{T^2}$$

over the temperature range 300 K< T < 1000 K.

a) Calculate ΔS if one mole of ethene is heated from 300 K to 600 K at constant volume.

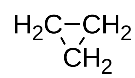
b) Calculate ΔS if one mole of ethene is heated from 300 K to 600 K at constant pressure. Assume ethane behaves ideally.

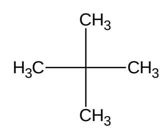
c) Compare and contrast the values from a) and b).

2. Why is $\Delta_{vap}S > \Delta_{fus}S$?

3. In each case below, predict which molecule of the pair has the greater molar entropy under the same conditions (assume gaseous species)? Justify your choices.

a) CO CO2

b) $CH_3CH_2CH_3$ 

c) $CH_3CH_2CH_2CH_2CH_3$ 

4. Use the data from McQuarrie and Simon problem 21-14 to show how you would calculate the standard molar entropy of N_2 at 298.15 K. (Just set up the math; don't solve it).

5. Using the partition function of a diatomic gas, an equation for the standard molar entropy can be determined. This is given as Equation 21.28 (Equations 21.22 to 21.27 show how Equation 21.28 was obtained).

a) Use Equations 21.28 and the data in Chapter 18 to calculate the standard molar entropy of CO(g) at its standard boiling point, 81.6 K.

b) Compare your answer from part 2b) with the experimental value of 155.6 $J \cdot K^{-1} \cdot mol^{-1}$. Why is there a discrepancy of about 5 $J \cdot K^{-1} \cdot mol^{-1}$?