Chem 205
Web problem set thermo-3

Question 1 :

The entropy of sublimation of certain compound is $\Delta S_{subl.}$ (J/K mol) at its normal sublimation point of $T_{subl.}$ ^{0}C. Calculate the vapor pressure in torr of the compound at T ^{0}C. Assume that the enthalpy of sublimation $\Delta H_{subl.}$ is constant.

Vapor pressure of the compound (in atm) can be easily calculated using Clausius-Clapeyron equation :

$$\ln\frac{p_2}{p_1} = -\frac{\Delta H_{subl}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$
$$\Delta H_{subl} = \Delta S_{subl.} T_{subl.} = \Delta S_{subl.} T_1$$

where P_2 is vapor pressure of compound at temperature T ($T=T_2$) and P_1 is vapor pressure of compound at temp. of sublimation $T_{subl.}$ ($T_{subl.}=T_1$),so P_1=1 atm.
In order to express the P_2 in torrs use conversion 1 atm=760 torr.

Question 2:

Compound	S^0 (J/K mol)
A	S^0_A
B	S^0_B
C	S^0_C
D	S^0_D

Delta G is ΔG^0 (kJ/mol) for the reaction

a A + b B ➔ c C + d D
Calculate ΔH^0 for the reaction in kJ.

From expression for ΔG^0 :

$$\Delta G^0 = \Delta H^0 - T\Delta S^0$$

ΔH^0 can be calculated as:

$$\Delta H^0 = \Delta G^0 + T\Delta S^0$$

where T=298 ^{0}K and

$$\Delta S^0 = \sum_f v_f S^0_f - \sum_i v_i S^0_i = (d \cdot S^0_D + c \cdot S^0_C) - (a \cdot S^0_A + b \cdot S^0_B)$$

Question 3 :

An important biochemical reaction that is used to do work (on muscle,or in transport of chemical species, or in driving biosynthesis) involves AdenosineTriPhosphate (ATP) and AdenosineDiPhosphate (ADP) and can be written as:

$ATP + H_2O \rightarrow ADP + Pi^{--} + H^+$

Delta G^0 = +9.2 kJ/mol
Where Pi^{--} is inorganic phosphate. In biological systems this reaction is, to an excellent approximation, carried out at constant pressure (1atm) and constant temperature.

Is this reaction spontaneous when carried out with all reactants and products present at standard state thermodynamic conditions?

a. yes,it is spontaneous with all reactants and products present at standard state conditions
b. no,it is not spontaneous with all reactants and products present at standard state thermodynamic conditions-it is spontaneous in the reverse direction
c. It is at equilibrium when all reactants and products are present at standard state thermodynamic conditions
d. The information given is not sufficient to answer the question

Answer : b

Starting from the general expression for delta G for the reaction :

$$\Delta G = \Delta G^0 - RT \ln Q = \Delta G^0 - RT \ln \frac{[ADP] \cdot [H^+] \cdot [Pi^{--}]}{[ATP]}$$ and appying the standard conditions for all reactants and products,delta G becomes :

$$\Delta G = \Delta G^0 > 0$$

Since delta G is greater that zero reaction is not spontaneous.

If reaction was in reverse direction then $\Delta G^0 = -7.2 kJ/mol$ and $\Delta G = \Delta G^0 < 0$,reaction would be spontaneous.

Question 4 :

Calculate Delta G in Joules for the ATP-ADP reaction of Question 5 at 25^0C and the typical physiological conditions:

PH = 7.2
[ATP] = 0.00025 M
[ADP] = 0.00011 M
$[Pi^{--}]$ = 0.0001 M

$$\Delta G = \Delta G^0 - RT \ln Q = \Delta G^0 - RT \ln \frac{[ADP] \cdot [H^+] \cdot [Pi^{--}]}{[ATP]}$$ where

$[H^+]$= -log pH

$\Delta G^0 = 7.2 kJ/mol$

T=298 K

Question 5 :

Is the ATP-ADP reaction in question 5 spontaneous under the conditions of question 6 ?

a. yes
b. no

If $\Delta G < 0$ then reaction is spontaneous (answer a) , if $\Delta G > o$ then reaction is not spontaneous (answer b).