Homework #4

1. Thermodynamics #1

Based on only the following information, determine the standard free energy change $^{\Delta}G°$ and K value at 25°C and 1 atm for the dissociation of carbonic acid, $H_2CO_3 = H^+ + HCO_3^-$.

Available information:

Reaction	K (@25°C, 1 atm)
$H_2CO_3 = CO_{2(aq)} + H_2O$	630

Species	$^{\Delta}G°_f$ (@25°C, 1 atm) (kJ/mol)
$CO_{2(aq)}$	-386.22
H_2O	-237.18
H^+	0.0
HCO_3^-	-586.85

2. Thermodynamics #2

Estimate the value of K_W at 20°C and 1 atm. Assume that at 25°C and 1 atm, the following is true:

Equation	Equilibrium Constant (K_w)
$H_2O = H^+ + OH^-$	1.01×10^{-14}

Species	$H°_f$ (kJ/mol)
H^+	0
OH^-	-230.0
H_2O	-285.83

3. Acid/Base Equilibria II: MINEQL method

Solve the problems from question #1 in homework #3 (1A and 1B copied below) using MINEQL[1]. Present the MINEQL-based concentrations in a table. Compare your MINEQL results with the approximate solutions you obtained from your graphs in problem homework #3 (note: when solving problems with the carbonate system, you will have to send aqueous CO_2 to the Type VI category just as you did for H^+. When we work with open carbonate systems, you won't have to do this.)

A). Consider a 0.10 F phosphate (H_3PO_4, $H_2PO_4^-$, HPO_4^{-2}, PO_4^{-3}) system. Using MINEQL, calculate the pH and the concentration of all species in the following solutions:

i) 0.10 F NaH_2PO_4
ii) 0.10 F Na_2HPO_4
iii) 0.10 F Na_3PO_4

[1] You may also use other chemical equilibria programs besides MINEQL, if you prefer. Examples of others include ChemEQL and MINTEQ.

B) Consider a 0.10 F carbonate system (H_2CO_3, HCO_3^-, CO_3^{-2}) and 0.20 F ammonia system (NH_4^+, NH_3), and use MINEQL to calculate pH and composition of the following systems:

i) 0.10 F $NaHCO_3$

ii) 0.10 F $NaHCO_3$ + 0.20 F NH_4Cl

iii) 0.10 F $(NH_4)_2CO_3$

iv) 0.10 F Na_2CO_3

Assigned: 26 Feb 20
Due: 4 Mar 20