WUCT: Individual Exam Sample

- 1. The air we breathe consists of mainly nitrogen and oxygen but also trace amounts of many other gases, such as carbon dioxide, helium, methane and hydrogen. For the purpose of this question, air can be approximated to be a system of three gases: nitrogen, oxygen and argon, with a total pressure of 1 atm and a temperature of 295 K.
 - a) Given that the mass percent of nitrogen, oxygen, and argon are 78%, 21%, and 1% respectively, answer the following questions.

i. Find the partial pressures of each gas.

78% of N₂
$$\rightarrow \frac{78\%}{28.02\frac{g}{mol}} = 2.784 \text{ mol }\%$$

21% of O₂ $\rightarrow \frac{21\%}{32\frac{g}{mol}} = 0.656 \text{ mol }\%$
1% of Ar $\rightarrow \frac{1\%}{39.95\frac{g}{mol}} = 0.025 \text{ mol }\%$

Total mol percent = 2.784 + 0.656 + 0.025 = 3.465 mol Mole fraction:

 N_2 : O_2 : Ar:

N2:

$$\frac{2.784 \text{ mol \%}}{3.465 \text{ mol}} \qquad \frac{0.656 \text{ mol \%}}{3.465 \text{ mol}} \qquad \frac{0.025 \text{ mol \%}}{3.465 \text{ mol}} \\= 0.803 = 0.189 = 0.00722$$

Dalton's law: partial pressure is mole fraction of total pressure (1 atm): N_2 : O_2 :Ar:= 0.803 atm= 0.189 atm= 0.00722 atm

ii. What are the densities of each gas in air? Density: (Due to the given temperature and pressure, the ideal gas law can be assumed valid)

$$PV = nRT \therefore \rho = \frac{m}{V} = \frac{n \cdot MW}{V} \therefore \rho = \frac{MW}{V} \cdot \frac{PV}{RT} = \frac{MW \cdot P}{RT}$$

where R = 0.08206 $\frac{L \ atm}{mol \ K}$ and T = 295 K
O2: Ar:

$$\frac{0.803 \ atm \cdot 28.02 \ \frac{g}{mol}}{0.08206 \ \frac{L \ atm}{mol \ K} \cdot 295 \ K} = 0.929 \ \frac{g}{L} = 0.250 \ \frac{g}{L} = 0.250 \ \frac{g}{L} = 0.0119 \ \frac{g}{L}$$

$$\frac{0.00722 \ atm \cdot 39.95 \ \frac{g}{mol}}{0.08206 \ \frac{L \ atm}{mol \ K} \cdot 295 \ K} = 0.0119 \ \frac{g}{L}$$

iii. What is the composition of air by volume?

Composition by volume = composition by mass divided by density, then normalized so they add up to 100%.

Except these densities should be the standard densities of each of the gases, where the pressure is equal to 1 Thus:

N2:
$$0.929 \frac{g}{L} \cdot \frac{1 \ atm}{0.803 \ atm} = 1.16 \frac{g}{L}$$

O2: $0.250 \frac{g}{L} \cdot \frac{1 \ atm}{0.189 \ atm} = 1.32 \frac{g}{L}$
Ar: $0.0119 \frac{g}{L} \cdot \frac{1 \ atm}{0.00722 \ atm} = 1.65 \frac{g}{L}$
N2: O2: Ar:

78%	21%	1%
$1.16\frac{g}{L}$	$\overline{1.32 \frac{g}{L}}$	$1.65 \frac{g}{L}$
= 67.4%	= 15.9%	= 0.606%

Notice that these percents do not add up to 100%, need to normalize them.

67.4% + 15.9% + 0.606% = 83.9%Multiply each percent by $\frac{100\%}{83.9\%}$: N2: O2: Ar: $67.4\% \cdot \frac{100\%}{83.9\%} = 15.9\% \cdot \frac{100\%}{83.9\%} = 0.606\% \cdot \frac{100\%}{83.9\%} = 0.722\%$

- b) A sample of air is placed in a 2 L container, with all other conditions the same.
 - i. How many moles of nitrogen are in the container? (Assume the partial pressure of nitrogen is 0.8 atm)

Use the ideal gas law: PV=nRT

$$n = \frac{PV}{RT} = \frac{0.8 \ atm \cdot 2 \ L}{0.08206 \frac{L \ atm}{mol \ K} \cdot 295 \ K} = 0.0661 \ moles$$

ii. If 0.5 moles of argon was added to the container how would the partial pressure of each gas change?

The partial pressure of nitrogen would not change because the addition of an inert gas to a container does not change the partial pressures of the other gas. The same applies to oxygen gas

The partial pressure of Argon would increase because according to Avogadro's law, increasing the moles would increase the pressure.

2. Any alkali metal upon addition to water would result in an explosive reaction. The weakest reaction would be the lithium with water reaction, while the cesium with water reaction is the most explosive. Lithium reacts with water according to the following reactions:

$$2 H_2O_{(1)} + 2e^- ----> H_{2(g)} + 2 OH_{(aq)} \qquad E^o = -0.83 V$$

Li⁺_(aq) + e⁻ ----> Li_(s)
$$E^o = -3.05 V$$

a) Write the overall **<u>balanced</u>** reaction of lithium with water and calculate the overall standard reduction potential.

2 Li(s) + 2 H₂O → 2 LiOH (aq) + H₂(g) With $E^{o} = -0.83$ V - (-3.05 V) = 2.22 V

b) If the reaction occurs at a pH of 9, calculate the equilibrium constant of the reaction at T = 295 K.

Reaction occurs at pH of 9, so $[OH^{-}] = \frac{10^{-14}}{10^{-9}} = 1 \cdot 10^{-5} M$ Have to use Nernst equation to calculate potential of the cell.

$$E = E^{\circ} - \frac{RT}{nF} \ln Q = 2.22 \text{ V} - \frac{8.314 \frac{J}{mol \, K} * 295 \, K}{2 \, mol \, * \, 96485 \, C/mol} * \ln([OH^{-}]^{2}) = 2.52 \text{ V}$$
$$E = \frac{RT}{nF} \cdot \ln \text{ K}$$
$$\ln \text{ K} = \frac{E * nF}{RT} = \frac{2.52 \, V * 2 \, mol \, * \, 96485 \, C/mol}{8.314 \frac{J}{mol \, K} * 295 \, K} = 198$$
$$\text{ K} = e^{198} = 9.09 * 10^{85}$$

3. Hydrogen gas is a popular clean alternative to fossil fuels and can be produced as either a primary product or coproduct from coal. In this production process, the H₂ to CO ratio must be adjusted for downstream process requirements, often accomplished by the water gas shift reaction:

$$CO(g) + H_2O(g) \rightleftharpoons H_2(g) + CO_2(g)$$

a. What is the equilibrium expression for this reaction, K_p ?

$$K_p = \frac{P_{H_2} P_{CO_2}}{P_{CO} P_{H_2O}}$$

b. 1.50 atm of CO and a certain amount of H₂O gas is added into a rigid evacuated 3.50 L container at 400.°C. If the equilibrium H₂ to CO mole ratio is 3:1, how many moles of H₂O gas was added into the container? (K_p = 12.0)

 $P_{CO_{initial}} = 1.5 atm$ $P_{H_2O_{initial}} = x atm$

$$CO(g) + H_2O(g) \rightleftharpoons H_2(g) + CO_2(g)$$

$$I \quad 1.5 \quad x \quad 0 \quad 0$$

$$C \quad -c \quad -c \quad +c \quad +c$$

$$E \quad 1.5-c \quad x-c \quad c \quad c$$

$$\frac{P_{H_2}}{P_{CO}} = \frac{c(atm)}{1.5-c(atm)} = 3.0$$

$$c = 1.125 \ atm$$

$$K_p = \frac{c^2(atm^2)}{(1.5-c)(x-c)(atm^2)} = \frac{1.125^2}{(1.5-1.125)(x-1.125)} = 12.0$$

$$x = 1.41 \ atm$$

$$n_{H_2O} = \frac{PV}{RT} = \frac{1.41(atm) \cdot 3.50(L)}{0.0821(L \cdot atm \cdot mol^{-1}K^{-1}) \cdot (273.15+400)(K)} = 8.91 \cdot 10^{-2} mol$$

c. What is the change in Gibbs Free Energy of the reaction?

$$\Delta G = -RT \ln(K) = -8.314 (J \cdot mol^{-1}K^{-1}) \cdot (273.15 + 400) (K) \ln(12.0) = -13.9 kJ$$

d. The standard entropy change for the water gas shift reaction is -42.26 J/K. Assuming the standard entropy change does not vary with temperature, calculate the enthalpy change of the reaction at 400.°C.

 $\Delta G = \Delta H - T\Delta S$ -13.9 (kJ) = $\Delta H - \frac{(273.15+400)(K)\cdot42.26(J/K)}{1000(J/kJ)}$ $\Delta H = -42.3 kJ$