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ALL work must be shown to receive full credit. **Due in lecture at 8:30 a.m. on Wednesday, March 13, 2002.**

PS7.1. Given the reaction

$$3O_{2(g)} + 4NH_{3(g)} \rightleftarrows 6H_2O_{(g)} + 2N_{2(g)}$$

Initially (before any reaction occurs) a 1.00 liter reaction vessel at 400 ˚C contains 0.502 moles of O_2 and 0.791 moles of NH_3 and no water or nitrogen. Consider the following:

a) If 0.0873 moles of O_2 react, how many moles of NH_3 must react and how many moles of H_2O and N_2 are formed? How many moles of O_2, NH_3, H_2O and N_2 remain after completion of the reaction?

	$3O_2$	$+ 4NH_3$	$\rightleftarrows 6H_2O$	$+ 2N_2$
initial	**.502**	**.791**	**0**	**0**
change	**-.0873**	**-.116**	**+.175**	**+.0582**
moles remaining(final)	**.415**	**.675**	**.175**	**.0582**

Note: the change row was determined using the reaction stoichiometry calculations below,

$$\mathbf{0.0873\ mol\ O_2\left(\frac{4\ mol\ NH_3}{3\ mol\ O_2}\right) = 0.116\ mol\ NH_3\ reacting}$$

$$\mathbf{0.0873\ mol\ O_2\left(\frac{6\ mol\ H_2O}{3\ mol\ O_2}\right) = 0.175\ mol\ H_2O\ formed}$$

$$\mathbf{0.0873\ mol\ O_2\left(\frac{2\ mol\ N_2}{3\ mol\ O_2}\right) = 0.0582\ mol\ N_2\ formed}$$

The moles remaining row is determined by adding the moles reacting or forming (change row) to the initial amount of each species.

b) If 0.234 moles of NH_3 react, how many moles of O_2 must react and how many moles of H_2O and N_2 are formed? How many moles of O_2, NH_3, H_2O and N_2 remain after completion of the reaction?

	$3O_2$	$+ 4NH_3$	$\rightleftarrows 6H_2O$	$+ 2N_2$
initial	**.502**	**.791**	**0**	**0**
change	**-.176**	**-.234**	**+.351**	**+.117**
moles remaining(final)	**.326**	**.557**	**.351**	**.117**

c) If '**3x**' moles of O_2 react, how many moles of NH_3 must react and how many moles of H_2O and N_2 are formed(in terms of '**x**')? How many moles of O_2, NH_3, H_2O and N_2 remain after completion of the reaction?

	$3O_2$	$+ 4NH_3$	$\rightleftarrows 6H_2O$	$+ 2N_2$
initial	**.502**	**.791**	**0**	**0**
change	**-3x**	**-4x**	**+6x**	**+2x**
moles remaining(final)	**.502-3x**	**.791-4x**	**0+6x**	**0+2x**

d) If 0.875 moles of H_2O are formed, how many moles of N_2 are formed and how many moles of O_2 and NH_3 must react? How many moles of O_2, NH_3, H_2O and N_2 remain after completion of the reaction?

	$3O_2$	$+ 4NH_3$	$\rightleftarrows 6H_2O$	$+ 2N_2$
initial	**.502**	**.791**	**0**	**0**
change	**-.438**	**-.583**	**+.875**	**+.292**
moles remaining(final)	**.064**	**.208**	**.875**	**.292**

PS7.2. Write the equilibrium expression for each of the following chemical equations;

a) $N_{2(g)} + O_{2(g)} \rightleftarrows 2NO_{(g)}$ $\quad K_c = \dfrac{[NO]^2}{[N_2]^1[O_2]^1}$ or $K_p = \dfrac{P^2_{NO}}{P^1_{N_2} \cdot P^1_{O_2}}$

b) $2NO_{(g)} + O_{2(g)} \rightleftarrows 2NO_{2(g)}$ $\quad K_c = \dfrac{[NO_2]^2}{[O_2]^1[NO]^2}$ or $K_p = \dfrac{P^2_{NO_2}}{P^1_{O_2} \cdot P^2_{NO}}$

c) $N_{2(g)} + 2O_{2(g)} \rightleftarrows 2NO_{2(g)}$ $\quad K_c = \dfrac{[NO_2]^2}{[N_2]^1[O_2]^2}$ or $K_p = \dfrac{P^2_{NO_2}}{P^1_{N_2} \cdot P^2_{O_2}}$

d) $2N_2O_{(g)} + O_{2(g)} \rightleftarrows 4NO_{(g)}$ $\quad K_c = \dfrac{[NO]^4}{[N_2O]^2[O_2]^1}$ or $K_p = \dfrac{P^4_{NO}}{P^2_{N_2O} \cdot P^1}$

PS7.3. Equilibrium constants for the following reactions have been determined at 550 ˚C:

$CoO_{(s)} + H_{2(g)} \rightleftarrows Co_{(s)} + H_2O_{(g)}$ $\quad K_1 = 67$

$CoO_{(s)} + CO_{(g)} \rightleftarrows Co_{(s)} + CO_{2(g)}$ $\quad K_2 = 490$

Calculate K (at the same temperature) for the commercially important water gas shift reaction

$H_2O_{(g)} + CO_{(g)} \rightleftarrows H_{2(g)} + CO_{2(g)}$ $\quad K_3 = ?$

$$\mathbf{Co_{(s)} + H_2O_{(g)} \rightleftarrows H_{2(g)} + CoO_{(s)}} \qquad \frac{1}{K_1} = .0149$$

$$\mathbf{CoO_{(s)} + CO_{(g)} \rightleftarrows Co_{(s)} + CO_{2(g)}} \qquad K_2 = 490$$

$$\mathbf{H_2O_{(g)} + CO_{(g)} \rightleftarrows H_{2(g)} + CO_{2(g)}} \qquad \left(\frac{1}{K_1}\right) \cdot K_2 = 7.30$$

PS7.4. Calculate K_c for the reaction

$$N_{2(g)} + O_{2(g)} \rightleftarrows 2NO_{(g)}$$

if K_c for the reaction

$$\frac{1}{2}N_{2(g)} + \frac{1}{2}O_{2(g)} \rightleftarrows NO_{(g)}$$

is 1.3×10^4.

$$\mathbf{K_c = \frac{[NO]^1}{[N_2]^{1/2}[O_2]^{1/2}} = 1.3 \times 10^4}$$

$$\mathbf{K_c' = \frac{[NO]^2}{[N_2]^1[O_2]^1} = (K_c)^2 = (1.3 \times 10^4)^2 = 1.7 \times 10^8}$$

PS7.5. A 1.00 liter container initially holds 0.257 moles of NOBr at a given temperature. The reaction which occurs is:

$$2NOBr_{(g)} \rightleftarrows 2NO_{(g)} + Br_{2(g)}$$

At equilibrium analysis shows 0.240 moles of NO and 0.120 moles of Br_2.

a) Which direction did the reaction proceed to establish (reach) equilibrium?

Reaction proceeds from left to right (L $\rightarrow$ R)

b) How many moles of NOBr reacted in order to form 0.240 moles of NO and 0.120 moles of Br_2?

If 0.240 mol of NO are formed in the reaction, then;

$$\textbf{0.240 mol NO}\left(\frac{\textbf{2 mol NOBr}}{\textbf{2 mol NO}}\right) = \textbf{0.240 mol NOBr reacted}$$

If 0.120 mol of Br_2 are formed in the reaction, then;

$$\textbf{0.120 mol Br}_2\left(\frac{\textbf{2 mol NOBr}}{\textbf{1 mol Br}_2}\right) = \textbf{0.240 mol NOBr reacted}$$

c) How many moles of NOBr remain after equilibrium was established?

$$[NOBr]_{eq} = [NOBr]_0 + [NOBr]_{reacted} = 0.257\ M - 0.240\ M$$

$$[NOBr]_{eq} = 0.017\ M$$

d) What is the magnitude of K_c?

$$K_c = \frac{[NO]^2[Br_2]}{[NOBr]^2} = \frac{[0.240]^2[0.120]}{[0.017]^2} = 23.9$$

PS7.6. In a container, the partial pressure of NOCl is initially 0.340 atm at a given temperature. The chemical equation which describes the reaction is:

$$2NO_{(g)} + Cl_{2(g)} \rightleftarrows 2NOCl_{(g)}$$

At equilibrium analysis shows the partial pressure of NO is 0.0916 atm.

a) Which direction did the reaction proceed to establish (reach) equilibrium?

Reaction proceeds from right to left (R $\rightarrow$ L)

b) What is the partial pressure of NOCl which reacted in order for the partial pressure of NO to be 0.0916 atm?

For the partial pressure of NO to be 0.0916 atm, the amount of NOCl which must react is,

$$\textbf{0.0916 atm NO}\left(\frac{\textbf{2 atm NOCl}}{\textbf{2 atm NO}}\right) = \textbf{0.0916 atm NOCl}$$

c) What is the partial pressure of Cl_2 at equilibrium?

Since the initial partial pressure of Cl_2 is zero, the amount of Cl_2 formed is equal to the amount at equilibrium.

$$\textbf{0.0916 atm NO}\left(\frac{\textbf{1 atm Cl}_2}{\textbf{2 atm NO}}\right) = \textbf{0.0458 atm Cl}_2$$

$$(P_{Cl_2})_{eq} = (P_{Cl_2})_0 + (P_{Cl_2})_{forming}$$

$$(P_{Cl_2})_{eq} = 0 + 0.0458\ atm = 0.0458\ atm$$

d) What is the partial pressure of NOCl at equilibrium?

$$(P_{NOCl})_{eq} = (P_{NOCl})_0 - (P_{NOCl})_{reacted}$$

$$(P_{NOCl})_{eq} = 0.340\ atm - 0.0916\ atm = 0.248\ atm$$

e) What is the magnitude of K_p?

$$K_p = \frac{P^2_{NOCl}}{P^2_{NO}\cdot P_{Cl_2}} = \frac{(0.248)^2}{(0.0916)^2(0.0458)} = 160$$

PS7.7. A 1.00 liter container holds 1.06 moles of H_2 and 1.57 moles of CO at a temperature of 162 ˚C. At this temperature, the following reaction occurs,

$$2H_{2(g)} + CO_{(g)} \rightleftarrows CH_3OH_{(g)}$$

After equilibrium is established, analysis shows 0.200 moles of CH_3OH in the container. Calculate the $[CO]_{eq}$, $[H_2]_{eq}$ and K_c.

	$2H_{2(g)}$ +	$CO_{(g)}$ ⇄	$CH_3OH_{(g)}$	
Initial	**1.06 M**	**1.57 M**	**0**	**let x = $[CO]_{reacting}$**
Change	**-2x**	**-x**	**+x**	
Equilibrium	**1.06 - 2x**	**1.57 - x**	**0 + x**	

$$[CH_3OH]_{eq} = 0.200\ M = x$$

$$[H_2]_{eq} = 1.06 - 2x = 1.06 - 2(0.2\ M) = 0.660\ M$$

$$[CO]_{eq} = 1.57 - x = 1.57 - (0.2\ M) = 1.37\ M$$

$$K_c = \frac{[CH_3OH]}{[H_2]^2[CO]} = \frac{(0.200)}{(0.660)^2 \cdot (1.37)} = 0.335$$

PS7.8. The following reaction,

$$2HI_{(g)} \rightleftarrows I_{2(g)} + H_{2(g)}$$

occurs at 298K. If 2.00 mol of HI are placed into a 1.00 liter container and permitted to react, at equilibrium it is found that 20.0 % of the HI has decomposed. Calculate K_c and K_p.

	2HI ⇄	H_2 +	I_2
initial	**2.00**	**0**	**0**
change	**-2x**	**+x**	**+x**
equilibrium	**1.60**	**+.2**	**+.2**

At equilibrium, 20% of the HI has decomposed; therefore, 0.20(2.0 M) = 0.4 M is the amount of HI that reacts.

0.4 M = 2x

0.2 M = x

Substituting

$$K_c = \frac{[H_2][I_2]}{[HI]^2} = \frac{(.2)(.2)}{(1.6)^2} = 0.0156$$

$$K_p = K_c = .0156$$

PS7.9 The equation which describes the preparation of ammonia is:

$$N_{2(g)} + 3H_{2(g)} \rightleftarrows 2NH_{3(g)}$$

A 3.000 L reaction vessel initially contains 0.3000 moles N_2 and 0.4500 moles H_2. When the reaction is allowed to attain equilibrium at a given temperature, analysis determines 0.09992 M N_2. Calculate K_c for the reaction.

	$N_{2(g)}$ +	$3H_{2(g)}$ $\rightleftarrows$	$2NH_{3(g)}$	
Initial	**0.1000 M**	**0.1500 M**	**0**	**let x = $[N_2]_{reacting}$**
Change	**-x**	**-3x**	**+2x**	
Equilibrium	**0.100 - x**	**0.150 - 3x**	**0 + 2x**	

$[N_2]_{eq}$ **= 0.1000 M - x = 0.09992 M**

x = 0.1000 M - 0.09992 M = 8 x 10^{-5} M

$[H_2]_{eq}$ **= 0.150 - 3x = 0.150 - 3(8 x 10^{-5} M) = 0.1498 M**

$[NH_3]_{eq}$ **= 2x = 2(8 x 10^{-5} M) = 1.6 x 10^{-4} M**

$$K_c = \frac{[NH_3]^2}{[N_2][H_2]^3} = \frac{(1.6 \times 10^{-4})^2}{(0.09992)(0.1498)^3} = 7.62 \times 10^{-5}$$