Chem Factsheet

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Calculating Equilibrium Compositions – A Cool Method!

When carrying out calculations to find equilibrium constants such as Kc and Kp, the first stage of the process is to calculate the overall composition of the equilibrium mixture in terms of the numbers of moles of each reactant and the numbers of moles of each product. This, unfortunately, often seems to present problems. This Factsheet is designed to help you overcome these hurdles.

A typical problem might be:

When 2.00 moles of hydrogen and 1.80 moles of iodine are mixed and allowed to reach equilibrium at constant temperature in a sealed vessel, the resulting mixture is found to contain 1.20 moles of hydrogen iodide. Calculate the overall composition of the equilibrium mixture.

> **Note:** Equilibrium is the state achieved when the rate of the forward reaction equals the rate of the backward reaction. This is a dynamic state where the numbers of moles of each reactant and each product reach constant values.

The aim of this problem is to calculate the number of moles of hydrogen, iodine and hydrogen iodide in the equilibrium mixture. The following procedure will allow you to do this for this and any other similar problem.

1. Write the balanced equation for the equilibrium reaction
   Equation $H_2 + I_2 \rightleftharpoons 2HI$

2. Insert the initial and equilibrium mole values that are known from the problem.

	H_2	+	I_2	⇌	2HI
***I**nitial*	2.00		1.80		0.00
***E**quilibrium*					1.20

3. Identify for which reactant or product you know *both* initial and equilibrium amounts. In this case it is hydrogen iodide (HI). Calculate the ***c**hange* in the number of moles this substance between initial and equilibrium conditions. Express it as a multiple of the coefficient for that substance in the equation. For HI, this is "2". This gives:

	H_2	I_2	2HI	
***I**nitial*	2.00	1.80	0.00	moles
***C**hange*			+2.00-1.20 = +0.80 =***2***(+0.40)	moles
***E**quilibrium*			1.20	moles

4. Complete the calculation by deducing the changes in the number of moles of the other reactants and products remembering that they *must occur in the same ratio as the numbers of moles in the balanced equation*. Also, there must be gains (+) on one side of the equation and losses (-) on the other. This gives:

	H_2	I_2	2HI	
***I**nitial*	2.00	1.80	0.00	moles
***C**hange*	= **1**(-0.40) = - 0.40	= **1**(-0.40) = - 0.40	+2.00-1.20 = +0.80 =***2*** (+0.40)	moles
***E**quilibrium*	= 2.00 – 0.40 = **1.60**	= 1.80 – 0.40 = **1.40**	**1.20**	moles

> **Notice** the initials of the three row labels; ICE. This gives a cool way of remembering the stages needed to successfully complete these sorts of problem!

Example 2

15.50g of phosphorus pentachloride (PCl_5) is heated at 500K in a sealed container. When equilibrium is reached, 4.56g of chlorine (Cl_2) is formed. Calculate the mole composition of the equilibrium mixture.

NB Make sure any mention of "grams" is first converted to moles

	PCl_5	PCl_3	Cl_2	
***I**nitial*	15.50/208.5 = 0.0743	0.00	0.00	mol
***C**hange*	= **1**(-0.0642) = -0.0642	= **1**(+0.0642) = +0.0642	0.0642 – 0.00 = +0.0642 = **1**(+0.0642)	mol
***E**qm*	= 0.0743 – 0.0642 = **0.0101**	= 0.00 +0.0642 = **0.0642**	4.56/71.0 = **0.0642**	mol

Example 3

0.856 moles of nitrogen (N_2) is mixed with 1.934 moles of hydrogen (H_2) and heated at 600K in a sealed container. When equilibrium is reached, 0.116 moles of ammonia (NH_3) is formed. Calculate the mole composition of the equilibrium mixture.

	N_2	$3H_2$	$2NH_3$	
***I**nitial*	0.856	1.934	0.00	mol
***C**hange*	= **1**(-0.0580) =-0.0580	= **3**(-0.0580) = -0.174	0.116 – 0.00 =+0.116 = **2**(+0.0580)	mol
***E**qm*	= 0.856 – 0.0580 = **0.798**	= 1.934 – 0.174 = **1.760**	= **0.116**	mol

Example 4

Substances A and B react to give C and D according to the following equation

$$2A + B \rightleftharpoons 3C + 2D$$

1.20 moles of A, 0.80 moles of B, 1.50 moles of C and 1.00 moles of D are mixed together and allowed to reach equilibrium at constant temperature in a sealed vessel. At equilibrium, 0.90 moles of C remain. Calculate the mole composition of the equilibrium mixture.

	2A	+ B	⇌ 3C	+ 2D	
*I*nitial	1.20	0.80	1.50	1.00	mol
*C*hange	= **2**(+0.20) = + 0.40	= **1**(+0.20) = + 0.20	= 0.90 – 1.50 = -0.60 = **3**(-0.20)	= **2**(-0.20) = -0.40	mol
*E*qm	= 1.20 + 0.40 = **1.60**	= 0.80 + 0.20 = **1.00**	**0.90**	= 1.00 – 0.40 = **0.60**	mol

Example 5

Sulphur dioxide (SO_2) and oxygen (O_2) are mixed together at 700K in a sealed vessel and allowed to reach equilibrium. The equilibrium mixture contained 1.22 moles of sulphur dioxide (SO_2), 0.84 moles of oxygen (O_2) and 1.66 moles of sulphur trioxide (SO_3). Calculate the numbers of moles of SO_2 and O_2 used initially.

NB *This example is the reverse of the previous ones. We are calculating from equilibrium back to initial*

	$2SO_2$	+ O_2	⇌ $2SO_3$	
*I*nitial	= 1.22 + 1.66 = **2.88**	= 0.84 + 0.83 = **1.67**	0.00	mol
*C*hange	= 2(-0.83) = -1.66	= **1**(-0.83) = -0.83	1.66 – 0.00 = +1.66 = **2**(+0.83)	mol
*E*qm	1.22	0.84	1.66	mol

Now try some similar examples for yourself.

Practice Questions

1. $CH_3COOH \rightleftharpoons CH_3COO^- + H^+$
   0.3840 moles of ethanoic acid (CH_3COOH) is added to water. When equilibrium is reached, 0.0025 moles of hydrogen ions (H^+) are formed. Calculate the mole composition of the equilibrium mixture.

2. $2NO_2 + 4CO \rightleftharpoons N_2 + 4CO_2$
   1.240×10^{-3} moles of nitrogen dioxide (NO_2) are mixed with 3.440×10^{-3} moles of carbon monoxide (CO). When equilibrium is reached, 4.640×10^{-4} moles of carbon dioxide (CO_2) are formed. Calculate the mole composition of the equilibrium mixture.

3. $CH_3COOH + CH_3OH \rightleftharpoons CH_3COOCH_3 + H_2O$
   0.828 moles of ethanoic acid (CH_3COOH) is mixed with 1.440 moles of methanol (CH_3OH). When equilibrium is reached, 0.444 moles of ethanoic acid (CH_3COOH) remain. Calculate the mole composition of the equilibrium mixture.

4. $4NH_3 + 5O_2 \rightleftharpoons 4NO + 6H_2O$
   1.824 moles of ammonia (NH_3) is mixed with 1.284 moles of oxygen (O_2), 1.112 moles of nitrogen monoxide (NO) and 0.826 moles of steam (H_2O). When equilibrium is reached, 0.528 moles of steam (H_2O) remain. Calculate the mole composition of the equilibrium mixture.

5. $CO + 2H_2 \rightleftharpoons CH_3OH$
   Carbon monoxide (CO) and hydrogen (H_2) are mixed together at 900K in a sealed vessel and allowed to reach equilibrium. The equilibrium mixture contained 2.46 moles of carbon monoxide (CO), 4.88 moles of hydrogen (H_2) and 1.18 moles of methanol (CH_3OH). Calculate the numbers of moles of carbon monoxide (CO) and hydrogen (H_2) used initially.

Answers

1. 0.3815 moles CH_3COOH, 0.0025 moles CH_3COO^- and 0.0025 moles H^+
2. 1.008×10^{-3} moles NO_2, 2.976×10^{-3} moles CO, 1.160×10^{-4} moles N_2 and 4.640×10^{-4} moles CO_2
3. 0.444 moles CH_3COOH, 1.056 moles CH_3OH, 0.384 moles CH_3COOCH_3 and 0.384 moles H_2O
4. 2.023 moles NH_3, 1.532 moles O_2, 0.913 moles NO and 0.528 moles H_2O
5. 3.64 moles CO and 7.24 moles H_2.

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