

EQUILIBRIUM

2: CALCULATING CONCENTRATIONS AT EQUILIBRIUM

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CALCULATING CONCENTRATIONS

Concentrations of chemicals can be calculated at equilibrium.

- ICE method is used for this where concentrations at different points of reaction are determined.
 - I = Initial concentration
 - C = Change of concentration during reaction
 - E = Equilibrium concentration

EXAMPLE 1: CALCULATING CONCENTRATION

When heated PCl_5 , phosphorus pentachloride, forms PCl_3 and Cl_2 as follows:



When 1.00 mol PCl_5 in a 1.00-L container is allowed to come to equilibrium at a given temperature, the mixture is found to contain 0.135 mol PCl_3 . What is the molar composition of the mixture?

Answer:

	$\text{PCl}_{5(g)} \rightleftharpoons$	$\text{PCl}_{3(g)} +$	$\text{Cl}_{2(g)}$
Initial (I)	1.00 mol	0	0
Change (C)	-x	+x	+x
Equilibrium (E)	$1.00 - x$	0.135 mol	x

We were told that the equilibrium amount of PCl_3 is 0.135 mol.

That means $x = 0.135$ mol.

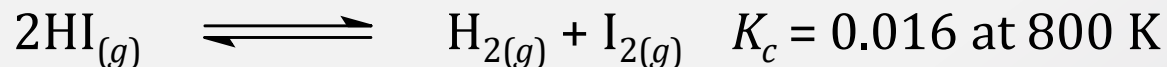
Moles $\text{PCl}_5 = 1.00 - 0.135 = 0.87$ mol

Moles $\text{PCl}_3 = 0.135$ mol

Moles $\text{Cl}_2 = 0.135$ mol

EXAMPLE 2: USING THE ICE METHOD

Hydrogen iodide decomposes to hydrogen gas and iodine gas.



If 0.50 mol HI is placed in a 5.0-L flask, what will be the composition of the equilibrium mixture in molarities?

Answer:

$$[\text{HI}]_0 = \frac{0.50 \text{ mol}}{5.0 \text{ L}} = 0.10 \text{ M}$$

	$2\text{HI}_{(g)} \rightleftharpoons$	$\text{H}_{2(g)} +$	$\text{I}_{2(g)}$
Initial	0.10 M	0	0
Change	$-2x$	$+x$	$+x$
Equilibrium	$0.10 - 2x$	x	x

The K_c expression is, $K_c = \frac{[\text{H}_2][\text{I}_2]}{[\text{HI}]^2}$

$$0.016 = \frac{[x][x]}{[0.10 - 2x]^2} = \frac{x^2}{(0.10 - 2x)^2}$$

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USING THE ICE METHOD... CONTD...

Because the right side of the equation is a perfect square, we can take the square root of both sides.

From previous slide:

$$0.016 = \frac{x^2}{(0.10 - 2x)^2}$$

$$\begin{aligned}\sqrt{0.016} &= \sqrt{\frac{x^2}{(0.10 - 2x)^2}} \\ 0.126 &= \frac{x}{(0.10 - 2x)}\end{aligned}$$

Solving:

$$0.126(0.10 - 2x) = x$$

$$0.0126 - 0.252x = x$$

$$0.0126 = 1.252x$$

$$x = 0.010 \text{ M}$$

Substituting:

$$[\text{H}_2] = [\text{I}_2] = x = 0.010 \text{ M}$$

$$[\text{HI}] = 0.10 - 2x = 0.10 - 0.020 = 0.08 \text{ M}$$

WHEN K_c EXPRESSION IS NOT SQUARE ROOT

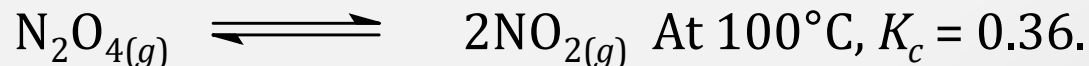
When the K_c expression is not a perfect square, the equation must be rearranged to fit the quadratic format:

$$ax^2 + bx + c = 0$$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

EXAMPLE 3: CALCULATING EQ CONC. 1

N_2O_4 decomposes to NO_2 . The equilibrium reaction in the gas phase is



If a 1.00-L flask initially contains 0.100 M N_2O_4 , what will be the equilibrium concentration of NO_2 ?

Answers:

	$\text{N}_2\text{O}_{4(g)} \rightleftharpoons$	$2\text{NO}_{2(g)}$
Initial	0.100 M	0
Change	-x	+2x
Equilibrium	0.100 - x	2x

The K_c expression is, $K_c = \frac{[\text{NO}_2]^2}{[\text{N}_2\text{O}_4]}$

$$0.36 = \frac{[2x]^2}{[0.100 - x]} = \frac{4x^2}{(0.100 - x)}$$

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EXAMPLE 3: CALCULATING EQ CONC. 1 CONTD....

From previous slide:

$$0.36 = \frac{4x^2}{(0.100 - x)}$$

Rearrange: (by cross multiplication) $4x^2 + 0.36x - 0.036 = 0$

$$ax^2 + bx + c = 0$$

$$a = 4 \quad b = 0.36 \quad c = -0.036$$

Substitute:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$x = \frac{-0.36 \pm \sqrt{(0.36)^2 - 4(4)(-0.036)}}{2(4)}$$

Solve:

$$x = \frac{-0.36 \pm \sqrt{0.7056}}{8}$$

$$x = -0.045 \pm 0.105$$

$$x = 0.06$$

$$x = -0.15$$

Substitute to find the equilibrium concentration of NO_2 :

$$[\text{NO}_2] = 2x = 2(0.06) = 0.12 \text{ M}$$

EXAMPLE 4: CALCULATING EQ CONC. 2

Given: $\text{H}_{2(g)} + \text{F}_{2(g)} \rightleftharpoons 2\text{HF}_{(g)}$; $K_c = 1.15 \times 10^2$

3.000 mol of each species is put in a 1.500-L vessel. What is the equilibrium concentration of each species?

Answer:

Calculate initial conc.: $[\text{H}_2]_0 = [\text{F}_2]_0 = [\text{HF}]_0 = \frac{3.000 \text{ mol}}{1.500 \text{ L}} = 2.000 \text{ M}$

	$\text{H}_{2(g)} +$	$\text{F}_{2(g)} \rightleftharpoons$	$2\text{HF}_{(g)}$
Initial	2.000 M	2.000 M	2.000 M
Change	-x	-x	+2x
Equilibrium	$2.000 - x$	$2.000 - x$	$2.000 + 2x$

$$K_c = \frac{[\text{HF}]^2}{[\text{H}_2][\text{F}_2]}$$

$$1.15 \times 10^2 = \frac{[2.000 + 2x]^2}{[2.000 - x]^2}$$

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EXAMPLE 4: CALCULATING EQ CONC. 2 CONTD.....

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$$\sqrt{1.15 \times 10^2} = \sqrt{\frac{[2.000 + 2x]^2}{[2.000 - x]^2}}$$

$$10.72 = \frac{[2.000 + 2x]}{[2.000 - x]}$$

$$10.72(2.000 - x) = (2.000 + 2x)$$

$$21.44 - 10.72x = 2.000 + 2x$$

$$19.44 = 12.72x$$

$$x = \frac{19.44}{12.72} = 1.528 \text{ M}$$

- Now compute the equilibrium concentrations:

$$[\text{H}_2] = [\text{F}_2] = 2.000 - x = 2.000 - 1.528 = 0.47 \text{ M}$$

$$[\text{HF}] = 2.000 + 2x = 2.000 + 3.06 = 5.06 \text{ M}$$

- You can do a cross - check:

$$K_c = \frac{[\text{HF}]^2}{[\text{H}_2][\text{F}_2]} = \frac{(5.06)^2}{(0.47)^2} = 1.16 \times 10^2$$

KEY CONCEPTS

- Calculate concentrations at equilibrium
- Be able to use the quadratic equation.