02/25/02

- Questions for today's Problem Session?
- Demo Wednesday!
- Quiz Friday!

The *ICE* Method

$$(CH_3)_2CHOH\ (g) \leftrightarrows (CH_3)_2CO\ (g) + H_2\ (g)$$

Initial:	0.3086 atm	-	-
Change:	**-x**	**+x**	**+x**
Equilibrium:	***0.3086 - x***	***x***	***x***

Plug values into equilibrium constant expression:

$$\mathbf{K = (P_{acet})(P_{H2})/(P_{isopro})}$$

Solving for x

$$K = \frac{(x)(x)}{0.3086 - x} = 0.444$$

It's a quadratic!

$$x^2 = 0.13702 - 0.444x$$

$$x^2 + 0.444x - 0.13702 = 0$$

a **b** **c**

$$x = \frac{-b \pm (b^2 - 4ac)^{1/2}}{2a}$$

Solving for x (continued)

- Substituting into the quadratic equation:

$$x = \frac{-0.444 \pm [(0.444)^2 - 4(1)(-0.13702)]^{1/2}}{2(1)}$$

- Rearranging and solving:

$$x = \frac{-0.444 \pm 0.863259}{2} = 0.20963$$

Negative root has no physical meaning

Relating x to pressures

- Substitute x back into equilibrium pressure expressions:

$P_{acetone} = P_{H2} = x =$ ***0.210 atm***

$P_{isopropanol} = 0.3086 - x =$ ***0.099 atm***

➢What is the *%-dissociation* of isopropanol?

%-dissoc = $(P_{reacted}/P_{initial}) \times 100$

$= (x/0.3086) \times 100$

$= (0.20963/0.3086) \times 100 =$ ***67.9%***

5

Disturbing Equilibrium

What happens when we *disturb* a system at equilibrium?

Le Chatelier's Principle:

Reaction will proceed so as to *counteract* the effects of the disturbance

Let's look at the effects of changing:

- Amount of a product or reactant
- Volume
- Pressure

6

Changing Amounts of Reactant or Product

Back to our example reaction:

$(CH_3)_2CHOH\ (g) \leftrightarrows (CH_3)_2CO\ (g) + H_2\ (g)$

- ➢ *Remove* a product: rxn shifts to the **right**
- ➢ **Add** a reactant: rxn shifts to the **right**

- ➢ *Remove* a reactant : rxn shifts to the **left**
- ➢ **Add** a product : rxn shifts to the **left**

7

Now, Quantitatively

- We start at our established point of equilibrium:

$P_{acetone} = P_{H2} =$ ***0.210 atm***

$P_{isopropanol} =$ ***0.099 atm***

➢What will the equilibrium pressures become IF we add H_2 so that:

$P_{H2} = 0.300$ atm?

8

ICE Again

$(CH_3)_2CHOH\ (g) \leftrightarrows (CH_3)_2CO\ (g) + H_2\ (g)$

$\longleftarrow$ ***Shift***

Initial:	0.0990 atm	0.210	0.300
Change:	**+x**	**-x**	**-x**
Equilibrium:	*0.0990* + *x*	*0.210* - *x*	*0.300* - *x*

9

Solve for x

$$K = \frac{(0.210 - x)(0.300 - x)}{0.0990 + x} = 0.444$$

From the quadratic formula, we get:

x = 0.0204

Substituting into *ICE* equilibrium expressions, gives:

$P_{isopropanol}$ = 0.0990 + x = $\boldsymbol{0.119\ atm = P_{isopropanol}}$

$P_{acetone}$ = 0.210 - x = $\boldsymbol{0.190\ atm = P_{acetone}}$

P_{H2} = 0.300 - x = $\boldsymbol{0.280\ atm = P_{H2}}$

10

Changing Volume

- Let's see what happens if we *halve* the volume of our reaction vessel:

$(CH_3)_2CHOH\ (g) \leftrightarrows (CH_3)_2CO\ (g) + H_2\ (g)$

At equilibrium:

0.119 atm   0.210 atm   0.280 atm

Halving the volume will **double** the pressures:

0.238 atm   *0.420 atm*   *0.560 atm*

What happened to Q?

11

Equilibrium Check!

$$Q = \frac{(0.420)(0.560)}{0.238} = 0.988$$

$$Q = 0.988 > 0.444 = K$$

Too much product, so reaction shifts:

$(CH_3)_2CHOH\ (g) \leftrightarrows (CH_3)_2CO\ (g) + H_2\ (g)$

$\longleftarrow$ ***Shift***

12

Volume Change: In General

- Changing the *volume* will change the partial pressures of all gases
  - ✓ If the ***number of moles of gas*** products or reactants is not the same, then the change in pressure will be different for the products and reactants (and Q ≠ K)
  - ✓ Equilibrium shifts to *decrease* the overall pressure and the reaction shifts to the side with the fewest number of moles of gas (until Q = K).
  - ✓ What ***if*** $\boldsymbol{\Delta n_{gas} = 0}$***? No Shift!*** (Q = K).

13