

## Chemistry 132 NT

Be true to your work,  
your word, and your  
friend.

Henry David Thoreau

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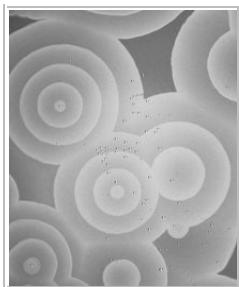
Chem 132 NT

## Chemical Equilibrium

### Module 2

Using the Equilibrium Constant

- Interpreting the Equilibrium Constant
- Predicting the Direction of a Reaction
- Calculating Equilibrium Concentrations



Oscillating patterns  
formed by a reaction  
far from equilibrium

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## Review

- Equilibrium and the **equilibrium constant,  $K_c$** .
- Obtaining equilibrium constants for reactions.
- The equilibrium constant,  **$K_p$** .
- Equilibrium constants for **sums of reactions**.
- Heterogeneous equilibrium.

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### Using the Equilibrium Constant

- ✦ In the last module, we looked at how a chemical reaction reaches **equilibrium** and how this equilibrium is characterized by an **equilibrium constant**.
- ◆ In this module, we will look at how we can use the equilibrium constant.

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### Using the Equilibrium Constant

- ✦ In the last module, we looked at how a chemical reaction reaches **equilibrium** and how this equilibrium is characterized by an **equilibrium constant**.
- We'll look at the following uses.
1. **Qualitatively interpreting the equilibrium constant .**

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## Using the Equilibrium Constant

- ✎ In the last module, we looked at how a chemical reaction reaches **equilibrium** and how this equilibrium is characterized by an **equilibrium constant**.

We'll look at the following uses.

### 2. Predicting the direction of a reaction.

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## Using the Equilibrium Constant

- ✎ In the last module, we looked at how a chemical reaction reaches **equilibrium** and how this equilibrium is characterized by an **equilibrium constant**.

We'll look at the following uses.

### 3. Calculating equilibrium concentrations.

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## Qualitatively Interpreting the Equilibrium Constant

- ✎ As stated in the last module, if the **equilibrium constant is large**, you know immediately that the products are favored at equilibrium.

◆ For example, consider the Haber process



At 25°C the equilibrium constant equals  $4.1 \times 10^8$ .

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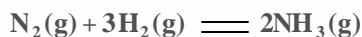
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### Qualitatively Interpreting the Equilibrium Constant

As stated in the last module, if the **equilibrium constant is large**, you know immediately that the products are favored at equilibrium.

- For example, consider the Haber process



In other words, at this temperature, the reaction **favors the formation of ammonia** at equilibrium.

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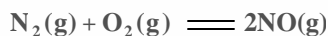
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### Qualitatively Interpreting the Equilibrium Constant

As stated in the last module, if the **equilibrium constant is small**, you know immediately that the reactants are favored at equilibrium.

- On the other hand, consider the reaction of nitrogen and oxygen to give nitric oxide, NO.



At 25°C the equilibrium constant equals  $4.6 \times 10^{-31}$ .

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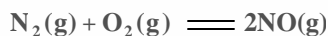
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### Qualitatively Interpreting the Equilibrium Constant

As stated in the last module, if the **equilibrium constant is small**, you know immediately that the reactants are favored at equilibrium.

- On the other hand, consider the reaction of nitrogen and oxygen to give nitric oxide, NO.



In other words, this reaction occurs to a **very limited extent**.

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## Predicting the Direction of Reaction

✎ How could one predict the direction in which a reaction at **non-equilibrium conditions** will shift to re-establish equilibrium?

◆ To answer this question, you substitute the current concentrations into the reaction quotient expression and compare it to  $K_c$ .

◆ The **reaction quotient,  $Q_c$** , is an expression that has the same form as the equilibrium-constant expression but whose concentrations are not necessarily at equilibrium.

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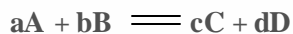
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## Predicting the Direction of Reaction

✎ For the general reaction



the  $Q_c$  expression would be:

$$Q_c = \frac{[C]_i^c [D]_i^d}{[A]_i^a [B]_i^b}$$

where the subscript “i” signifies initial or current concentrations.

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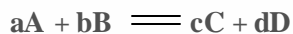
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## Predicting the Direction of Reaction

✎ For the general reaction



the  $Q_c$  expression would be:

$$Q_c = \frac{[C]_i^c [D]_i^d}{[A]_i^a [B]_i^b}$$

◆ If  $Q_c > K_c$ , the reaction will shift left... toward reactants.

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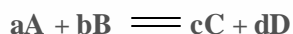
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## Predicting the Direction of Reaction

✎ For the general reaction



the  $Q_c$  expression would be:

$$Q_c = \frac{[C]_i^c [D]_i^d}{[A]_i^a [B]_i^b}$$

- ✦ If  $Q_c < K_c$ , the reaction will shift right... toward products.

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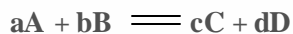
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## Predicting the Direction of Reaction

✎ For the general reaction



the  $Q_c$  expression would be:

$$Q_c = \frac{[C]_i^c [D]_i^d}{[A]_i^a [B]_i^b}$$

- ✦ If  $Q_c = K_c$ , the reaction is at equilibrium and will not shift.

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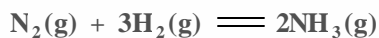
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## A Problem To Consider

✦ Consider the following equilibrium.



- ✦ A 50.0 L vessel contains 1.00 mol  $N_2$ , 3.00 mol  $H_2$ , and 0.500 mol  $NH_3$ . In which direction (toward reactants or toward products) will the system shift in order to reestablish equilibrium at 400 °C?
- ✦ The  $K_c$  for the reaction at 400 °C is 0.500.

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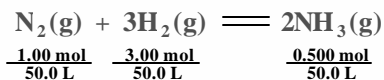
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### A Problem To Consider

- First, calculate concentrations from moles of substances.



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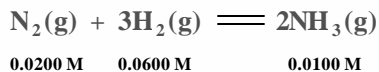
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### A Problem To Consider

- First, calculate concentrations from moles of substances.



- The  $Q_c$  expression for the system would be:

$$Q_c = \frac{[\text{NH}_3]^2}{[\text{N}_2][\text{H}_2]^3}$$

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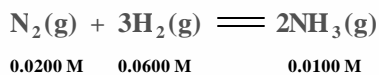
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### A Problem To Consider

- First, calculate concentrations from moles of substances.



- Substituting these concentrations into the reaction quotient gives:

$$Q_c = \frac{(0.0100)^2}{(0.0200)(0.0600)^3} = 23.1$$

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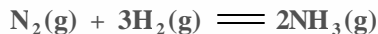
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### A Problem To Consider

- ◆ First, calculate concentrations from moles of substances.



0.0200 M    0.0600 M            0.0100 M

- ◆ Because  $Q_c = 23.1$  is greater than  $K_c = 0.500$ , the **reaction will go to the left (toward reactants)** as it approaches equilibrium.

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### Calculating Equilibrium Concentrations

- ◆ Once you have determined the equilibrium constant for a reaction, you can use it to **calculate the concentrations of substances in the equilibrium mixture.**

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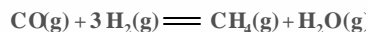
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### Calculating Equilibrium Concentrations

- ◆ For example, consider the following equilibrium.



- ◆ Suppose a gaseous mixture contained 0.30 mol CO, 0.10 mol  $\text{H}_2$ , 0.020 mol  $\text{H}_2\text{O}$  and an unknown amount of  $\text{CH}_4$  per liter.
- ◆ What is the concentration of the  $\text{CH}_4$  in this mixture? The equilibrium constant  $K_c$  equals 3.92.

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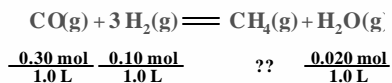
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## Calculating Equilibrium Concentrations

- First, calculate concentrations from moles of substances.



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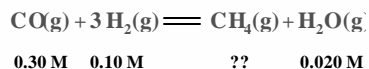
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## Calculating Equilibrium Concentrations

- First, calculate concentrations from moles of substances.



- The equilibrium-constant expression is:

$$K_c = \frac{[\text{CH}_4][\text{H}_2\text{O}]}{[\text{CO}][\text{H}_2]^3}$$

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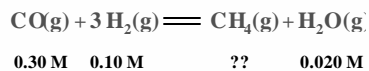
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## Calculating Equilibrium Concentrations

- First, calculate concentrations from moles of substances.



- Substituting the known concentrations and the value of  $K_c$  gives:

$$3.92 = \frac{[\text{CH}_4](0.020\text{M})}{(0.30\text{M})(0.10\text{M})^3}$$

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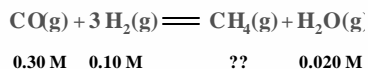
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### Calculating Equilibrium Concentrations

- First, calculate concentrations from moles of substances.



- You can now solve for  $[\text{CH}_4]$ .

$$[\text{CH}_4] = \frac{(3.92)(0.30\text{M})(0.10\text{M})^3}{(0.020\text{M})} = 0.059$$

- The concentration of  $\text{CH}_4$  in the mixture is **0.059 mol/L**.

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### Calculating Equilibrium Concentrations

- Suppose we begin a reaction with known amounts of starting materials and want to **calculate the quantities at equilibrium?**

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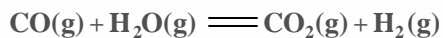
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### Calculating Equilibrium Concentrations

- Consider the following equilibrium.



- Suppose you start with 1.000 mol each of carbon monoxide and water in a 50.0 L container. Calculate the molarities of each substance in the equilibrium mixture at 1000 °C.
- The  $K_c$  for the reaction is 0.58 at 1000 °C.

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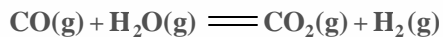
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## Calculating Equilibrium Concentrations

- First, calculate the initial molarities of CO and H<sub>2</sub>O.



$$\frac{1.000 \text{ mol}}{50.0 \text{ L}} \quad \frac{1.000 \text{ mol}}{50.0 \text{ L}}$$

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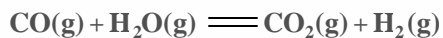
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## Calculating Equilibrium Concentrations

- First, calculate the initial molarities of CO and H<sub>2</sub>O.



$$0.0200 \text{ M} \quad 0.0200 \text{ M} \quad 0 \text{ M} \quad 0 \text{ M}$$

- The starting concentrations of the products are 0.
- We must now set up a table of concentrations (starting, change, and equilibrium expressions in x).

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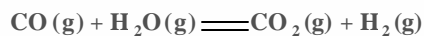
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## Calculating Equilibrium Concentrations

- Let x be the moles per liter of product formed.



Starting	0.0200	0.0200	0	0
Change	-x	-x	+x	+x
Equilibrium	0.0200-x	0.0200-x	x	x

- The equilibrium-constant expression is:

$$K_c = \frac{[\text{CO}_2][\text{H}_2]}{[\text{CO}][\text{H}_2\text{O}]}$$

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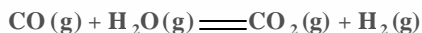
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## Calculating Equilibrium Concentrations

♦ Solving for x.



Starting	0.0200	0.0200	0	0
Change	-x	-x	+x	+x
Equilibrium	0.0200-x	0.0200-x	x	x

♦ Substituting the values for equilibrium concentrations, we get:

$$0.58 = \frac{(x)(x)}{(0.0200 - x)(0.0200 - x)}$$

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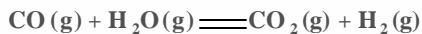
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## Calculating Equilibrium Concentrations

♦ Solving for x.



Starting	0.0200	0.0200	0	0
Change	-x	-x	+x	+x
Equilibrium	0.0200-x	0.0200-x	x	x

♦ Or:

$$0.58 = \frac{x^2}{(0.0200 - x)^2}$$

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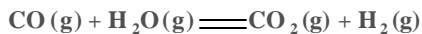
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## Calculating Equilibrium Concentrations

♦ Solving for x.



Starting	0.0200	0.0200	0	0
Change	-x	-x	+x	+x
Equilibrium	0.0200-x	0.0200-x	x	x

♦ Taking the square root of both sides we get:

$$\sqrt{0.58} = \sqrt{\frac{x^2}{(0.0200 - x)^2}}$$

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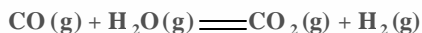
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## Calculating Equilibrium Concentrations

◆ Solving for x.



Starting	0.0200	0.0200	0	0
Change	-x	-x	+x	+x
Equilibrium	0.0200-x	0.0200-x	x	x

◆ Taking the square root of both sides we get:

$$0.76 = \frac{x}{(0.0200 - x)}$$

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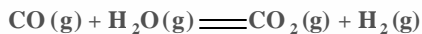
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## Calculating Equilibrium Concentrations

◆ Solving for x.



Starting	0.0200	0.0200	0	0
Change	-x	-x	+x	+x
Equilibrium	0.0200-x	0.0200-x	x	x

◆ Rearranging to solve for x gives:

$$x = \frac{0.0200 \cdot 0.76}{1.76} = 0.0086$$

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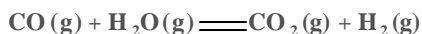
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## Calculating Equilibrium Concentrations

◆ Solving for equilibrium concentrations.



Starting	0.0200	0.0200	0	0
Change	-x	-x	+x	+x
Equilibrium	0.0200-x	0.0200-x	x	x

◆ If you substitute for x in the last line of the table you obtain the following equilibrium concentrations.

0.0114 M CO            0.0086 M CO<sub>2</sub>  
 0.0114 M H<sub>2</sub>O        0.0086 M H<sub>2</sub>

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## Calculating Equilibrium Concentrations

☛ The preceding example illustrates the three steps in solving for equilibrium concentrations.

1. **Set up a table** of concentrations (starting, change, and equilibrium expressions in x).
2. **Substitute the expressions in x** for the equilibrium concentrations into the equilibrium-constant equation.
3. **Solve the equilibrium-constant equation** for the values of the equilibrium concentrations.

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## Calculating Equilibrium Concentrations

☛ In some cases it is necessary to solve a **quadratic equation** to obtain equilibrium concentrations.

- ◆ Remember, that for the general quadratic equation:

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

the roots are defined as:

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

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## Calculating Equilibrium Concentrations

☛ In some cases it is necessary to solve a **quadratic equation** to obtain equilibrium concentrations.

- ◆ Remember, that for the general quadratic equation:

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

- ◆ The next example illustrates how to solve such an equation.

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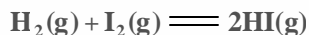
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## Calculating Equilibrium Concentrations

◆ Consider the following equilibrium.



◆ Suppose 1.00 mol  $\text{H}_2$  and 2.00 mol  $\text{I}_2$  are placed in a 1.00-L vessel. How many moles per liter of each substance are in the gaseous mixture when it comes to equilibrium at 458 °C?

◆ The  $K_c$  at this temperature is 49.7.

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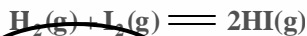
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## Calculating Equilibrium Concentrations

◆ The concentrations of substances are as follows.



Starting	1.00	2.00
Change	-x	-x
Equilibrium	1.00-x	2.00-x

0
+2x
2x

◆ The equilibrium-constant expression is:

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

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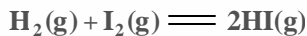
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## Calculating Equilibrium Concentrations

◆ The concentrations of substances are as follows.



Starting	1.00	2.00
Change	-x	-x
Equilibrium	1.00-x	2.00-x

0
+2x
2x

◆ Substituting our equilibrium concentration expressions gives:

$$49.7 = \frac{(2x)^2}{(1.00 - x)(2.00 - x)}$$

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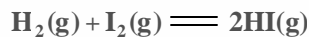
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## Calculating Equilibrium Concentrations

♦ Solving for x.



Starting	1.00	2.00	0
Change	-x	-x	+2x
Equilibrium	1.00-x	2.00-x	2x

♦ Because the right side of this equation is not a perfect square, you must solve the quadratic equation.

$$49.7 = \frac{(2x)^2}{(1.00 - x)(2.00 - x)}$$

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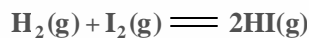
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## Calculating Equilibrium Concentrations

♦ Solving for x.



Starting	1.00	2.00	0
Change	-x	-x	+2x
Equilibrium	1.00-x	2.00-x	2x

♦ The equation rearranges to give:

$$0.920x^2 - 3.00x + 2.00 = 0$$

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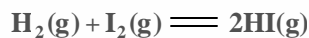
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## Calculating Equilibrium Concentrations

♦ Solving for x.



Starting	1.00	2.00	0
Change	-x	-x	+2x
Equilibrium	1.00-x	2.00-x	2x

♦ The two possible solutions to the quadratic equation are:

$$x = 2.33 \quad \text{and} \quad x = 0.93$$

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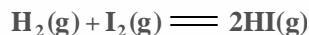
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## Calculating Equilibrium Concentrations

◆ Solving for x.



Starting	1.00	2.00	0
Change	-x	-x	+2x
Equilibrium	1.00-x	2.00-x	2x

◆ However,  $x = 2.33$  gives a negative value to  $1.00-x$  (the equilibrium concentration of  $\text{H}_2$ ), which is not possible.

**only  $x = 0.93$  remains**

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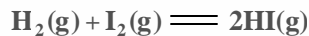
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## Calculating Equilibrium Concentrations

◆ Solving for equilibrium concentrations.



Starting	1.00	2.00	0
Change	-x	-x	+2x
Equilibrium	1.00-x	2.00-x	2x

◆ If you substitute 0.93 for x in the last line of the table you obtain the following equilibrium concentrations.

**0.07 M  $\text{H}_2$       1.07 M  $\text{I}_2$       1.86 M HI**

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## Operational Skills

- ✎ Using the reaction quotient,  $Q_c$
- ✎ Obtaining one equilibrium concentration given the others.
- ✎ Solving equilibrium problems

**Time for a few review questions.**

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