Date: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

**Solving Equilibrium Problems**

**Reaction Quotient (Q) vs. Equilibrium Constant (K)**

|  |  |
| --- | --- |
| **Similar** | **Different** |
| * Calculated in similar way

For aA + bB ⇌ cC,$$K= \frac{\left[C\right]c}{\left[A\right]a\left[B\right]b }$$$$Q= \frac{\left[C\right]c}{\left[A\right]a\left[B\right]b }$$ | * K is calculated using equilibrium concentrations
* K is a constant for a given temperature
* **K tells you where the system is going to end up**
 | * Q is calculated using instantaneous concentrations
* Q is not constant – many values of Q can be calculated for a system, depending on instantaneous concentrations
* **Q tells you where the system is**
 |

*The value of K*

K tells you to what extent the forward reaction proceeds to completion.

|  |  |
| --- | --- |
| **Value of K** | **Means…** |
| K << 1 | Reaction does not proceed to completion. Reactants are favoured. |
| K = 1 | At equilibrium, reactant and product concentrations are about equal. |
| K >> 1 | Reaction proceeds to completion. Products are favoured. |

*Comparing Q to K*

* If Q = K, the system is already at equilibrium
* If Q does NOT equal K, the system is not at equilibrium. It will shift until it reaches an equilibrium position.
	+ Q < K – Too many reactants, not enough products. System will shift right.
	+ Q > K – Too many products. System will shift left.

**Using ICE tables to solve equilibrium problems**

ICE tables are a visual way of laying out all of the information that you are provided, in order to solve an equilibrium problem. Here are some guidelines for ICE tables:

* ICE tables work with CONCENTRATIONS, in mol/L.
	+ You may be given concentrations, or you may be given molar amounts and volumes, in order to find concentrations.
* The rows in an ICE table represent the following:
	+ **Initial concentration** – This information is usually provided
	+ **Change in concentration** – You will need to figure this out for all species, in terms of a change *x*
	+ **Equilibrium concentration** – May be given; BUT you will usually have to express this algebraically using the Initial concentration, and the Change in concentration

***Scenario 1:***

|  |  |  |  |
| --- | --- | --- | --- |
| GIVEN   | All initial concentrations Equilibrium concentration of ONE species | REQUIRED | Equilibrium concentrations of all speciesOR Value of K |

**Example**. 0.600 mol of H2 and 0.600 mol of I2 are placed in a 1.00 L container. At equilibrium, the concentration of HI is measured as 0.960 mol/L.

H2 (g) + I2 (g) ⇌ 2 HI (g)

1. Determine the equilibrium concentrations of H2 and I2
2. Find the value of K at this temperature

Problem-Solving Logic:

The starting concentration of HI is 0 mol/L. Therefore, we know that the reaction will proceed to the right.

*Equilibrium concentrations of reactants*

In the process, a concentration of H2 will be consumed. Let us represent this unknown concentration algebraically with the variable *x.*

Therefore, at equilibrium, [H2]eq = (0.600 – *x*) mol/L

Since H2 and I2 react in a 1:1 ratio, the same concentration, *x*, of I2 will also be consumed.

This gives us [I2]eq = (0.600 – *x*) mol/L

*Equilibrium concentrations of products*

From the balanced equation, we know that, for every 1 mole of H2 reacted, 2 moles of HI are produced. It follows that the increase in concentration of HI will be equal to 2*x*.

Therefore, at equilibrium, [HI]eq = (0.000 + 2*x*) mol/L

Putting this information in an ICE table gives the following:

|  |  |  |  |
| --- | --- | --- | --- |
|  | **H2 (g)** | **I2 (g)**  | **2 HI (g)** |
| Initial concentration (M) | 0.600 | 0.600 | 0 |
| Change in concentration (M) | - *x* | - *x* | + 2*x* |
| Equilibrium concentration (M) |  |  | 0.960(given in question) |

General Strategy:

1. Let “x” = the change in concentration per 1 mole of your substances.
2. Use the balanced equation to write expressions for the change in concentration of each substance.
3. Solve for x.
4. Find unknown concentrations.

Solution:

a) Determine the equilibrium concentrations of H2 and I2

With the information we now have, we can solve for *x*, which represents the change in concentration of H2 and I2. Once *x* is found, solve for equilibrium concentrations of H2 and I2.

|  |  |  |
| --- | --- | --- |
| [HI]eq = 0 + 2*x* = 0.960 mol/Lx = 0.480 mol/L | [H2]eq = 0.600 - *x* = 0.120 mol/L | [I2]eq = 0.600 - *x* = 0.120 mol/L |

b) Find the value of K at this temperature

$$K = \frac{\left[HI\right]2}{\left[H2\right]\left[I2\right] } = \frac{0.9602}{(0.120)(0.120) }= 64.0$$

***Scenario 2.a: When K equation is a perfect square***

|  |  |  |  |
| --- | --- | --- | --- |
| GIVEN   | All initial concentrationsValue of K | REQUIRED | Equilibrium concentrations of all species |

In this scenario, you are going to have to use some fancy math tricks to find the value of *x*, since you are not given the equilibrium concentration. Without the equilibrium concentration, finding *x* is not as straightforward.

**Example**. 0.400 mol each of H2 and I2 are placed into a 2.00-L reaction chamber. At this specific temperature, K = 55.6. Determine the equilibrium concentrations of each species in the reaction chamber.

H2 (g) + I2 (g) ⇌ 2 HI (g)

Problem-Solving Logic

First off, pay some attention! You aren’t given the initial concentrations so you will have to find them.

[H2]0 = [I2]0 = $\frac{0.400 mol}{2.00 L}$ = 0.200 mol/L

Again in this scenario, we are starting with no product. This means that the reaction will proceed to the right. Using the same logic as in Scenario 1, we can express the changes in concentration and the equilibrium concentrations as shown in the ICE table.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **H2 (g)** | **I2 (g)**  | **2 HI (g)** |
| Initial concentration (M) | 0.200 | 0.200 | 0 |
| Change in concentration (M) | - *x* | - *x* | + 2*x* |
| Equilibrium concentration (M) | 0.200 - *x* | 0.200 - *x* | 2*x* |

|  |  |
| --- | --- |
| Now that you have expressions for all species’ equilibrium concentrations, you can **use the value of K to solve for *x.***Once *x* is found, you can solve for the equilibrium concentrations of each species. | $$K = \frac{\left[HI\right]2}{\left[H2\right]\left[I2\right] } $$$$55.6 = \frac{(2x)2}{(0.200 - x)(0.200 - x) }$$ |

Solution

|  |  |
| --- | --- |
| *Find* x$K = \frac{\left[HI\right]2}{\left[H2\right]\left[I2\right] } $ *sub in eqb’m [ ]expressions* $55.6 = \frac{(2x)2}{(0.200 - x)(0.200 - x) }$This equation looks complicated, but notice that it’s actually a perfect square! That means we can simplify this equation by taking the square root of both sides.$$\sqrt{55.6} = \sqrt{\frac{(2x)2}{(0.200 - x)(0.200 - x) }}$$$$7.457 = \frac{2x}{0.200 - x }$$7.457 (0.200 – *x*) = 2*x*1.491 – 7.457*x* = 2*x*1.491 = 9.457*x*0.158 mol/L = *x* (rounded to 3 SD) | *Find equilibrium concentrations*Don’t lose sight of what *x* represents. It represents the *change* in concentration. We still have to go back and sub this value in to find the equilibrium concentrations of each species.[H2]eq = 0.200 - *x* = 0.042 mol/L[I2]eq = 0.200 - *x* = 0.042 mol/L[HI]eq = 2*x* = 0.316 mol/LGeneral Strategy:1. Set up ICE table with all knowns.
2. Use balanced equation to represent changes in concentration, in terms of *x*.
3. In K expression, sub in K value, and algebraic expressions for equilibrium concentrations.
4. Solve for x.
5. Find values of equilibrium concentrations.
 |

***Scenario 2.b: When K equation is NOT a perfect square***

**Example**. 0.400 mol each of H2 and 0.300 mol of I2 are placed into a 2.00-L reaction chamber, along with 0.200 mol of HI. At this specific temperature, K = 55.6. Determine the equilibrium concentrations of each species in the reaction chamber.

H2 (g) + I2 (g) ⇌ 2 HI (g)

Problem-Solving Logic

It should strike you now that for the first time we are seeing a problem where there is an initial concentration of the product. So we first have to figure out: is the system already at equilibrium? If it’s not, how will it reach equilibrium – by shifting right to make more products, or by shifting left to make more reactants? You will have to calculate Q to figure this out.$Q = \frac{\left[HI\right]2}{\left[H2\right]\left[I2\right] } $ *sub in given concentrations* $Q = \frac{\left(0.200\right)2}{\left(0.200\right)\left(0.150\right)} $

Q = 1.33

Since Q < K, the system is not at equilibrium, and it will have to shift right in order to reach equilibrium. This means that the reactant concentrations will decrease, and the product concentration will increase.

Once we know HOW the concentrations will change, we can construct an ICE table:

|  |  |  |  |
| --- | --- | --- | --- |
|  | **H2 (g)** | **I2 (g)**  | **2 HI (g)** |
| Initial concentration (M) | 0.200 | 0.150 | 0.200 |
| Change in concentration (M) | - *x* | - *x* | + 2*x* |
| Equilibrium concentration (M) | 0.200 - *x* | 0.150 - *x* | 2*x* |

Solution

*Find* x

$K = \frac{\left[HI\right]2}{\left[H2\right]\left[I2\right] } $ *sub in* $55.6 = \frac{(2x)2}{(0.200 - x)(0.150 - x) }$

Since we don’t have a perfect square this time, we have to solve this the complicated way: expand the quadratic in the denominator, collect like terms, and solve for *x.*

$55.6 = \frac{4x^{2}}{(0.0300 - 0.350x + x^{2}) }$

$$55.6 (0.0300 - 0.350x + x^{2}) = 4x^{2}$$

1.668 -19.46*x* + 55.6*x*2 = 2*x*2

51.6*x*2 – 19.46*x* + 1.668 = 0 *(collect and re-arrange)*

To solve for *x*, we will need to use the quadratic formula, which tells us that for a quadratic equation in the form **a***x*2 + **b***x* + **c** = 0,

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

From our equation, a = 51.6, b = (-19.46), c = 1.668

Therefore

$$x=\frac{-(-19.46)\pm \sqrt{(-19.46)^{2}-4(51.6)(1.668)}}{2(51.6)}$$

Solving for x gives us two values:

*x*1 = 0.245 mol/L and *x*2 = 0.132 mol/L

Since *x* represents the change in concentration, and the initial concentration of *x*1 is larger than the initial concentration of both H2 and I2, ***x*1 cannot be the solution**. This means that **the correct solution is**
***x*2 = 0.132 mol/L**.

*Lastly, find equilibrium concentrations*

|  |  |  |
| --- | --- | --- |
| [H2]eq = 0.200 - *x* = 0.068 mol/L (rounded to 2 decimals) | [I2]eq = 0.150 - *x* = 0.018 mol/L | [HI]eq = 2*x* = 0.264 mol/L |

***Scenario 2.c: When K is very very tiny, and the math is so complicated that we need to make a simplifying assumption***

**Example**. 0.250 mol of CO2 is placed in a closed 1.00-L container and heated to 2000°C. At this temperature, K is 6.40 x 10-7. Find the equilibrium concentrations of all species.

2 CO2 (g) ⇌ 2 CO (g) + O2 (g)

Problem-Solving Logic

There are no initial concentrations of reactants. Therefore we know the reaction will proceed to the right.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **2 CO2 (g)** | **2 CO (g)**  | **O2 (g)** |
| Initial concentration (M) | 0.250 | 0 | 0 |
| Change in concentration (M) | - 2*x* | + 2*x* | + *x* |
| Equilibrium concentration (M) | 0.250 - 2*x* | 2*x* | *x* |

Constructing an ICE table and setting up our K expression gives us the following:

This is a cubic expression that is very difficult to solve.

$$K = \frac{\left[CO\right]2\left[O2\right]}{\left[CO2\right]2 }$$

(*sub in)* $6.40 ×10^{-7} = \frac{(2x)2(x)}{(0.250 - x)^{2} }= \frac{4x3}{(0.250 - x)^{2} }$

In order to simplify our calculations, we can recognize that the value of K is very small in comparison to the initial concentration of CO2. *Qualitatively*, this means that **very little CO2 will end up decomposing** into the products. We can therefore expect that the value of *x* will be exceedingly small, and that 2*x* won’t be much bigger.

*Quantitatively*, this means that when this small value is subtracted from the much larger value of 0.250, the result will essentially remain 0.250. With this knowledge, we can **make the simplifying assumption that 0.250 – 2x** ≅  **0.250**

Feeling uneasy about this? Don’t worry - at the end of the solution, we will validate this assumption using something called the “**hundred rule**”.

Solution

*Apply the simplifying assumption*

Make the statement:
 “Assume that 0.250 – x ≅ 0.250.”

*Find* x

NOTE: Even though we went ahead and solved this equation by using the simplifying assumption, you should always validate using the hundred rule BEFORE applying the assumption.

$K = \frac{\left[CO\right]2\left[O2\right]}{\left[CO2\right]2 } $ *sub in* $6.40 ×10^{-7} ≅  \frac{4x3}{(0.250)^{2} }$

4*x*3 ≅  4.00 x 10-8

*x* ≅  $\sqrt[3]{1.00×10^{-8}}$

*x* ≅  2.15 x 10-3mol/L

General Strategy:

1. Set up ICE table and K expression.
2. Use the **hundred rule** to see if a simplifying assumption is valid.
3. If valid, make your assumption statement.
4. Apply the assumption and solve for *x.*
5. Find equilibrium concentrations.

*Validate the simplifying assumption*

Before proceeding to calculate the equilibrium concentrations using the value of *x*, we need to make sure that the simplifying assumption was valid.

To do this, we use the “hundred rule”: **If the concentration to which *x* is added or subtracted is at least 100 times the value of K, the simplifying assumption can be made.**

$\frac{\left[CO\_{2}\right]^{2}}{K}=\frac{0.250}{6.40×10^{-7}}$

= 3.91 × 105

Since 3.91 × 105 > 100, the assumption that
(0.250 – 2*x*) ≅ 0.250 is warranted.

*Find equilibrium concentrations*

[CO2]eq = 0.250 - 2*x* = 0.248 mol/L

[CO]eq = 2*x* = 4.30 × 10-3 mol/L

[O2]eq = *x* = 2.15 × 10-3 mol/L