To determine the shift, we use the **reaction quotient**, ***Q***. The reaction quotient is obtained by applying the law of mass action using initial concentrations instead of equilibrium concentrations.

$$N_{2\,(g)} + 3\,H_{2\,(g)} \rightleftharpoons 2\,NH_{3\,(g)} \qquad Q = \frac{[NH_3]^2}{[N_2]\,[H_2]^3}$$

To determine in which direction a reaction will shift to reach equilibrium, we compare the values of Q and K.

1. Q is equal to K. The system is in equilibrium.
2. Q is greater than K. The system will shift to the left (toward the reactants)
3. Q is less than K. The system will shift to the right (toward the products)

$Q = K;$	at equilibrium
$Q > K;$	shift to the left
$Q < K;$	shift to the right

Example:

Calculate the reaction quotient (Q) for the following reaction at a specific temperature:

$N_{2\,(g)} + 3\,H_{2\,(g)} \rightleftharpoons 2\,NH_{3\,(g)}$, where:

$[\,N_2\,] = 4.6 \times 10^{-1}$ mol L^{-1}

$[\,H_2\,] = 2.2 \times 10^{-1}$ mol L^{-1}

$[\,NH_3\,] = 6.3 \times 10^{-1}$ mol L^{-1}

$$Q = \frac{[NH_3]^2}{[N_2][H_2]^3} = \frac{(6.3\times10^{-1})^2}{(4.6\times10^{-1})(2.2\times10^{-1})^3} = \boxed{81.0}$$

Example #2:

Calculate the reaction quotient (Q) for the following reaction at a specific temperature:

$2\,NH_{3\,(g)} \rightleftharpoons N_{2\,(g)} + 3\,H_{2\,(g)}$ where:

$[\,N_2\,] = 4.6 \times 10^{-1}$ mol L^{-1}

$[\,H_2\,] = 2.2 \times 10^{-1}$ mol L^{-1}

$[\,NH_3\,] = 6.3 \times 10^{-1}$ mol L^{-1}

$$Q = \frac{[N_2][H_2]^3}{[NH_3]^2} = \frac{(4.6\times10^{-1})(2.2\times10^{-1})^3}{(6.3\times10^{-1})^2} = \boxed{0.012}$$

We can draw a conclusion from the two examples (hopefully). If a reaction proceeds in the reverse direction under the same conditions the new equilibrium expression can be written as:

$$c\,\mathrm{C} + d\,\mathrm{D} \rightleftharpoons a\,\mathrm{A} + b\,\mathrm{B}$$

$$Q' = \frac{[A]^a\,[B]^b}{[C]^c\,[D]^d} = \frac{1}{Q}$$

Equilibrium Position:

Again, the equilibrium concentrations will not always be the same, but the equilibrium constant (K) remains the same at a given temperature. Using the data from the first example (front of the page) the conditions at equilibrium

$N_{2\,(g)} + 3\,H_{2\,(g)} \rightleftharpoons 2\,NH_{3\,(g)}$, where:

Initial concentrations	Equilibrium concentrations
$[\,N_2\,]_0 = 4.7 \times 10^{-1}$ mol L^{-1}	$[\,N_2\,] = 4.6 \times 10^{-1}$ mol L^{-1}
$[\,H_2\,]_0 = 2.9 \times 10^{-1}$ mol L^{-1}	$[\,H_2\,] = 2.2 \times 10^{-1}$ mol L^{-1}
$[\,NH_3\,]_0 = 0$ mol L^{-1}	$[\,NH_3\,] = 6.3 \times 10^{-1}$ mol L^{-1}

Each set of equilibrium concentrations is a called an equilibrium position (there can be an infinite number of positions) but only one equilibrium constant (K) for a given temperature. Look at the graph on the front side and pick any point in time (before equilibrium) that represents an equilibrium position.