10.3: Calculating Equilibrium Values

The numeric value of the equilibrium constant tells us something about the *ratio* of the reactants and products in the final equilibrium mixture. Likewise, the magnitude of the equilibrium constant tells us about the actual composition of that mixture.

In the three equilibrium systems, the first depicts a reaction in which the ratio of products to reactants is very *small*. Because the expression for the equilibrium constant is given by the pressure (or concentration) of products divided by the pressure (or concentration) of reactants, the equilibrium constant, *K*, for this system is also small. In the second example, the concentrations of reactants and products are shown to be *equal*, making the ratio (the equilibrium constant) equal to "1". In the last example, the products are shown to dominate the equilibrium mixture, making the ratio $(P_{Products})/(P_{Reactants})$ very large. In these examples, the stoichiometric ratios of the reactants and products are one and there is only one reactant and only one product; if multiple reactants or products are involved, the relationship between their concentrations would be more complex, but that ratio is always given by the expression for *K*. This fact allows us to take data for an equilibrium reaction and, if *K* is known, calculate concentrations for reactants and products. Likewise, if all of the equilibrium concentrations are known, we can use these to calculate a value for the equilibrium constant.

In these types of problems, an ICE table is often useful. This table has entries for *Initial* concentrations (or pressures), *Equilibrium* concentrations and any *Change* between the initial and equilibrium states. For example, consider the reaction between carbon monoxide and chlorine to form phosgene, a deadly compound that was used as a gas warfare agent in World War I.

$$CO\ (g) + Cl_2\ (g) \rightleftarrows COCl_2\ (g)$$

Example 10.3.1:

A mixture of CO and Cl_2 has initial partial pressures of 0.60 atm for CO and 1.10 atm for Cl_2. After the mixture reaches equilibrium, the partial pressure of $COCl_2$ is 0.10 atm. Determine the value of *K*.

Solution

The initial pressures for carbon monoxide and chlorine are placed in the first row and the equilibrium pressure for phosgene is placed in the last row. ***Initially***, the pressure of phosgene was zero, so that goes in the first row; the change for phosgene is therefore "+ 0.10 atm".

Solutions to Example 10.3.1

	P_{CO}	P_{Cl_2}	P_{COCl_2}
=== Initial ===	0.60 atm	1.10 atm	0 atm
Change			

+ 0.10 atm

Equilibrium

0.10 atm

Because one mole of CO is required to make one mole of $COCl_2$ the partial pressure of CO must have dropped by 0.10 atm (the ***Change***) in order to make $COCl_2$ with a partial pressure of 0.10 atm, giving a final (***Equilibrium***) pressure of 0.50 atm for carbon monoxide. Likewise, one mole of chlorine is required to make one mole of $COCl_2$ making the ***Change*** for chlorine 0.10 atm and the ***Equilibrium*** partial pressure 1.00 atm. The completed table is shown below:

Solutions to Example 10.3.1

	P_{CO}	P_{Cl_2}	P_{COCl_2}
=== Initial ===	0.60 atm	1.10 atm	0 atm
Change	-0.10 atm	-0.10 atm	+ 0.10 atm
Equilibrium	0.50 atm	1.00 atm	0.10 atm

The equilibrium expression for the phosgene-forming reaction is given by the following equation:

$$\frac{P_{COCl_2}}{P_{CO}P_{Cl_2}} = K$$

Substituting the values from the Table into this equation:

$$\frac{P_{COCl_2}}{P_{CO}P_{Cl_2}} = \frac{(0.10)}{(0.50)(1.00)} = 0.20$$

Notice that equilibrium constants for gas phase reactions are not typically written with units, although units are sometimes used in equilibrium constants calculated from molar concentrations. Many textbooks differentiate between equilibrium constants calculated from partial pressures and molar concentrations by affixing subscripts; K_P and K_C. In this book, we will simply use K and K_C to represent the two; a value for K will always denote a constant calculated from partial pressure data.

? Exercise 10.3.1

1. For the reaction shown below, all four gasses are introduced into a vessel, each with an initial partial pressure of 0.500 atm, and allowed to come to equilibrium; at equilibrium, the partial pressure of SO_3 is found to be 0.750 atm. Determine the value of *K*.

   $$\mathbf{SO_2\ (g) + NO_2\ (g) \rightleftarrows SO_3\ (g) + NO\ (g)}$$

2. For the reaction shown above, the initial partial pressures of SO_3 and NO are 0.500 atm under conditions where the equilibrium constant is, $K = 9.00$. The equilibrium partial pressure for SO_2 is found to be 0.125 atm. Calculate the equilibrium partial pressure for SO_3.