1.7: Chemical Equilibrium and Predicting Chemical Change

When we talk about predicting chemical reactions, we imagine taking quantities of various pure compounds and mixing them under some set of conditions. We suppose that they react until they reach a position of equilibrium in which one or more new compounds are present. We want to predict what these new compounds are and how much of each will be produced.

For any given set of reactants, we can accomplish this predictive program in two steps. First we find all of the sets of products that can be obtained from the given reactants. Each such set represents a possible reaction. We suppose that, for each set of possible products, we are able to predict the equilibrium composition. Predicting which reaction will occur is equivalent to finding the reaction whose position of equilibrium lies farthest in the direction of its products. From this perspective, being able to predict the position of equilibrium for the reactants and any stoichiometrically consistent set of products is the same thing as being able to predict what reaction will occur. (If there is no single reaction whose position of equilibrium is much further in the direction of its products than that of any other reaction, multiple reactions can occur simultaneously.)

This two-step procedure corresponds to the sense in which chemical thermodynamics enables us to predict reaction products. We measure values for certain characteristic thermodynamic functions for all relevant compounds. Given the values of these functions for all of the compounds involved in a hypothesized reaction, we calculate the position of equilibrium. That we must begin by guessing the products makes this approach cumbersome and uncertain. We can never be positive that the true products are among the possibilities that we consider. Nevertheless, as a practical matter for most combinations of reactants, the number of plausible product sets is reasonably small.