13.8: Predicting the Direction of a Reaction

Often you will know the concentrations of reactants and products for a particular reaction and want to know whether the system is at equilibrium. If it is not, it is useful to predict how those concentrations will change as the reaction approaches equilibrium. A useful tool for making such predictions is the **reaction quotient**, Q. Q has the same mathematical form as the equilibrium-constant expression, but Q is a ratio of the actual concentrations (not a ratio of equilibrium concentrations).

For example, suppose you are interested in the reaction

$$2\mathrm{SO_2}(g) + \mathrm{O_2}(g) \rightleftharpoons 2\mathrm{SO_3}(g)$$

$$K_\mathrm{c} = \frac{[\mathrm{SO_3}]^2}{[\mathrm{SO_2}]^2[\mathrm{O_2}]} = 245\ \mathrm{mol/L}(\mathrm{at}\ 1000\ \mathrm{K})$$

and you have added 0.10 mol of each gas to a container with volume 10.0 L. Is the system at equilibrium? If not, will the concentration of SO_3 be greater than or less than 0.010 mol/L when equilibrium is reached? You can answer these questions by calculating Q and comparing it with K_c. There are three possibilities:

- If $Q = K_c$ then the actual concentrations of products (and of reactants) are equal to the equilibrium concentrations and the system is at equilibrium.
- If $Q < K_c$ then the actual concentrations of products are less than the equilibrium concentrations; the forward reaction will occur and more products will be formed.
- If $Q > K_c$ then the actual concentrations of products are greater than the equilibrium concentrations; the reverse reaction will occur and more reactants will be formed.

For the reaction given above,

$$Q = \frac{[\mathrm{SO_3}]^2}{[\mathrm{SO_2}]^2[\mathrm{O_2}]} = \frac{(\frac{0.1mol}{10L})^2}{(\frac{0.1mol}{10L})^2(\frac{0.1mol}{10L})} = 100\frac{\mathrm{mol}}{\mathrm{L}}$$

(In the expression for Q each actual concentration is enclosed in braces {curly brackets} in order to distinguish it from the equilibrium concentrations, which, in the K_c expression, are enclosed in [square brackets].) In this case Q = 100 mol/L. This is less than K_c, which has the value 245 mol/L. This implies that the concentrations of products are less than the equilibrium concentrations (and the concentrations of reactants are greater than the equilibrium concentrations). Therefore the reaction will proceed in the forward direction, producing more products, until the concentrations reach their equilibrium values.

Example 13.8.1: Equilibrium

At 2300 K, the equilibrium constant, K_c, is 1.7 x 10^{-3} for the reaction

$$\mathrm{N_2}(g) + \mathrm{O_2}(g) \rightleftharpoons 2\mathrm{NO}(g)$$

A mixture of the three gases at 2300 K has these concentrations, $[N_2]$ = 0.17 mol dm^{-3}, $[O_2]$ = 0.17 mol dm^{-3}, and [NO] = 0.034 mol dm^{-3}.
(a) Is the system at equilibrium?
(b) In which direction must the reaction occur to reach equilibrium?
(c) What are the equilibrium concentrations of N_2, O_2, and NO?

Solution

Use the known concentrations to calculate Q. Compare Q with K_c to answer questions (a) and (b). Use an ICE table to answer part (c).

$$Q = \frac{\{\mathrm{NO}\}^2}{\{\mathrm{N_2}\}\{\mathrm{O_2}\}} = \frac{(0.034\mathrm{mol\ dm^{-3}})^2}{(0.17\mathrm{mol\ dm^{-3}})(0.17\mathrm{mol\ dm^{-3}})} = 4.0 \times 10^{-2}$$

a. Q is larger than K_c, so the reaction is not at equilibrium.

b. Because Q is larger than K_c, the concentration of the product, NO, is larger than its equilibrium concentration and the concentrations of the reactants, N_2 and O_2, are smaller than their equilibrium concentrations. Therefore some of the product, NO, will be consumed and more of the reactants, N_2 and O_2, will be formed.

c. Use the given concentrations as the initial concentrations of reactants and product. Enter these into an ICE table. Let x be the increase in the concentration of N_2 as the system reacts to equilibrium. The ICE table looks like this:

	N_2	O_2	NO
Initial concentration/mol dm^{-3}	0.17	0.17	0.034
Change in concentration/mol dm^{-3}	x	x	$-2x$
Equilibrium concentration/mol dm^{-3}	$0.17 + x$	$0.17 + x$	$0.034 - 2x$

Next, substitute the equilibrium concentrations into the K_c expression and solve for x.

$$K_c = 1.7 \times 10^{-3} = \frac{(0.034 - 2x)^2}{(0.17 + x)(0.1 + x)}$$

Now take the square root of both sides of this equation. This gives

$$\sqrt{1.7 \times 10^{-3}} = 0.0412 = \frac{0.034 - 2x}{0.17 + x}$$

Multiplying both sides by $0.17 + x$ gives

$$0.0070 + 0.412x = 0.034 - 2x$$

$$2x + 0.0412x = 0.034 - 0.0070$$

$$x = \frac{0.0270}{2.0412} = 0.0132$$

$$[N_2] = [O_2] = 0.17 + 0.013 = 0.183 \text{ mol dm}^{-3}$$

$$[NO] = 0.034 - 2(0.0132) = 0.0076 \text{ mol dm}^{-3}$$

Check the result by substituting these concentrations into the equilibrium constant expression.

$$K_c = \frac{(0.0076)^2}{(0.18)(0.18)} = 1.8 \times 10^{-3}$$

This agrees to two significant figures with the K_c value of 1.7×10^{-3}.