Key for Take-Home Assigment 05

In our last class session we considered the reaction

$$PCl_3(g) + Cl_2(g) \rightleftharpoons PCl_5(g)$$

for which the equilibrium constant expression is

$$K = \frac{[PCl_5]}{[PCl_3][Cl_2]}$$

Beginning with a system in which the initial concentrations of PCl_3, Cl_2, and PCl_5 were set to 0.0220 M, 0.00400 M, and 0.0400 M, respectively, and at a temperature where $K = 1000$, we determined equilibrium concentrations of 0.0201 M, 0.00209 M, and 0.0419 M for PCl_3, Cl_2, and PCl_5, respectively.

Suppose you start with a system in which the initial concentrations of PCl_3, Cl_2, and PCl_5 are 0.0508 M, 0.0108 M, and 0.1237 M, respectively, and at a temperature where the equilibrium constant has a value of 0.210. What are the concentrations of PCl_3, Cl_2, and PCl_5 at equilibrium? For this problem, apply the rigorous approach in which you use the quadratic equation. You may, if you wish, check your work using your calculator's solver function. For now, do not use the method that relies on a simplifying assumption; we will return to this approach later. Your sample number is 119.

This assignment is due in class on Monday.

Answer. Generally, it is a good idea to determine the direction in which the reaction must move to reach equilibrium so that when we solve for x, the chemically meaningful result is a positive number. To do this, we calculate Q

$$Q = \frac{[PCl_5]}{[PCl_3][Cl_2]} = \frac{0.1237}{0.0508 \times 0.0108} = 225$$

and note that as $Q > K$, the reaction must shift to the left to reach equilibrium; thus

$$K = \frac{[PCl_5]_o - x}{([PCl_3]_o + x)([Cl_2]_o + x)} = \frac{0.1237 - x}{(0.0508 + x)(0.0108 + x)} = 0.210$$

Rearranging into a second-order polynomial form gives

$$0.210x^2 + 1.013x + -0.124 = 0$$

Solving for the roots using the quadratic formula yields results for x of 0.1191 and -4.9426. The chemically meaningful result is the one that yields only positive concentrations for the reactants and products; in this case this is 0.1191 and the equilibrium concentrations are 0.0046, 0.1699, and 0.1299 for PCl_5, PCl_3, and Cl_2, respectively. To check this result, we substitute back into the equilibrium constant expression, finding that

$$K = \frac{[PCl_5]}{[PCl_3][Cl_2]} = \frac{0.0046}{0.1699 \times 0.1299} = 0.210$$