

Section 13.4

Equilibrium Calculations



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Learning Objectives



- Identify the changes in concentration or pressure that occur for chemical species in equilibrium systems
- Calculate equilibrium concentrations or pressures and equilibrium constants, using various algebraic approaches

Calculating Equilibrium Constant

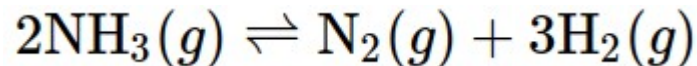


- Equilibrium constants are calculated from the equilibrium concentrations of reactants and products.
- If equilibrium concentrations are known, they can simply be substituted into the K expression
- If less information is available, you may need to make an ICE table to calculate the equilibrium concentration.

Representing Changes in Concentration



- Representing changes in concentration can be done using an ICE table.

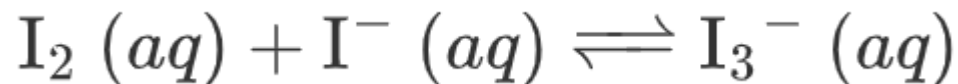


	$[\text{NH}_3]$	$[\text{N}_2]$	$[\text{H}_2]$
Initial Concentration	$[\text{NH}_3]_i$	$[\text{N}_2]_i$	$[\text{H}_2]_i$
Change	$-2x$	$+x$	$+3x$
Equilibrium Concentration	$[\text{NH}_3]_i - 2x$	$[\text{N}_2]_i + x$	$[\text{H}_2]_i + 3x$

K_c Calculation Example



- Iodine molecules react reversibly with iodide ions to produce triiodide ions.



If a solution with the concentrations of I_2 and I^- both equal to $1.000 \times 10^{-3} \text{ M}$ before reaction gives an equilibrium concentration of I_2 of $6.61 \times 10^{-4} \text{ M}$, what is the equilibrium constant for the reaction?

K_c Calculation Example



	I_2	+	I^-	\rightleftharpoons	I_3^-
Initial concentration (M)	1.000×10^{-3}		1.000×10^{-3}		0
Change (M)	$-x$		$-x$		$+x$
Equilibrium concentration (M)	$1.000 \times 10^{-3} - x$		$1.000 \times 10^{-3} - x$		x

- At equilibrium the concentration of I_2 is 6.61×10^{-4} M so

$$1.000 \times 10^{-3} \text{ M} - x = 6.61 \times 10^{-4} \text{ M}$$

$$x = 3.39 \times 10^{-4} \text{ M}$$

K_c Calculation Example



- The ICE table may now be updated with numerical values for all its concentrations

	I_2	+	I^-	\rightleftharpoons	I_3^-
Initial concentration (M)	1.000×10^{-3}		1.000×10^{-3}		0
Change (M)	-3.39×10^{-4}		-3.39×10^{-4}		$+3.39 \times 10^{-4}$
Equilibrium concentration (M)	6.61×10^{-4}		6.61×10^{-4}		3.39×10^{-4}

K_c Calculation Example



- Finally, substitute the equilibrium concentrations into the K expression and solve

$$K_c = \frac{[\text{I}_3^-]}{[\text{I}_2][\text{I}^-]}$$
$$= \frac{3.39 \times 10^{-4} \text{ M}}{(6.61 \times 10^{-4} \text{ M})(6.61 \times 10^{-4} \text{ M})} = 776$$

Missing Equilibrium Concentration Example



Nitrogen oxides are air pollutants produced by the reaction of nitrogen and oxygen at high temperatures. At 2000 °C, the value of the K_c for the reaction, $\text{N}_2(g) + \text{O}_2(g) \rightleftharpoons 2\text{NO}(g)$, is 4.1×10^{-4} . Calculate the equilibrium concentration of $\text{NO}(g)$ in air at 1 atm pressure and 2000 °C. The equilibrium concentrations of N_2 and O_2 at this pressure and temperature are 0.036 M and 0.0089 M, respectively.

Missing Equilibrium Concentration Example



$$K_c = \frac{[\text{NO}]^2}{[\text{N}_2][\text{O}_2]}$$

$$[\text{NO}]^2 = K_c[\text{N}_2][\text{O}_2]$$

$$[\text{NO}] = \sqrt{K_c[\text{N}_2][\text{O}_2]}$$

$$= \sqrt{(4.1 \times 10^{-4})(0.036 \text{ M})(0.0089 \text{ M})} = 3.6 \times 10^{-4} \text{ M}$$

Equilibrium Concentrations from Initial Concentrations



- The most challenging type of equilibrium calculation can be one in which equilibrium concentrations are derived from initial concentrations and an equilibrium constant.
- For these calculations, a four-step approach is used
 - 1) Identify the direction in which the reaction will proceed to reach equilibrium.
 - 2) Develop an ICE table.
 - 3) Calculate the concentration changes and, subsequently, the equilibrium concentrations.
 - 4) Confirm the calculated equilibrium concentrations.

Equilibrium Concentration Example



- Under certain conditions, the equilibrium constant K_c for the decomposition of $\text{PCl}_5(g)$ into $\text{PCl}_3(g)$ and $\text{Cl}_2(g)$ is 0.0211. What are the equilibrium concentrations of PCl_5 , PCl_3 , and Cl_2 in a mixture that initially contained only PCl_5 at a concentration of 1.00 M?

Step One



- Determine the direction the reaction proceeds.



- Because only the reactant is present initially $Q_c = 0$, which is less than K_c . Therefore the reaction will proceed to the right.

Step Two



- Develop an ICE table.

	$\text{PCl}_5 \rightleftharpoons \text{PCl}_3 + \text{Cl}_2$		
Initial concentration (M)	1.00	0	0
Change (M)	$-x$	$+x$	$+x$
Equilibrium concentration (M)	$1.00 - x$	x	x

Step Three



- Substituting the equilibrium concentrations into the equilibrium constant equation gives

$$K_c = \frac{[\text{PCl}_3][\text{Cl}_2]}{[\text{PCl}_5]}$$

$$= \frac{(x)(x)}{(1.00 - x)} = \frac{x^2}{(1.00 - x)} = 0.0211$$

$$x^2 = 0.0211(1.00 - x) = 0.0211 - 0.0211x$$

$$x^2 + 0.0211x - 0.0211 = 0$$

$$x = 0.135 \quad \text{or} \quad -0.156$$

Step Three Continued



- We can now substitute x into our concentration expressions.

$$[\text{PCl}_5] = 1.00 - x = 1.00 - 0.135 = 0.87 \text{ M}$$

$$[\text{PCl}_3] = x = 0.135 \text{ M}$$

$$[\text{Cl}_2] = x = 0.135 \text{ M}$$

Step Four



- To check the calculation, substitution the concentrations expression for K_c .

$$K_c = \frac{[\text{PCl}_3][\text{Cl}_2]}{[\text{PCl}_5]} = \frac{(0.135)(0.135)}{0.87} = 0.021$$

Approximations

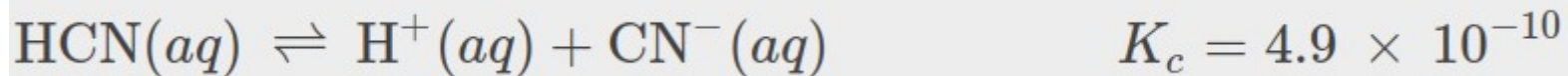


- When the change in concentration (x) is significantly less than the initial concentration the initial concentration experiences a negligible change.
 - This is a consequence of the small K value
- When these conditions are met, a clever approximation can be used.

Approximation Example



- What are the concentrations at equilibrium of a 0.15 M solution of HCN?



	$\text{HCN}(aq) \rightleftharpoons \text{H}^+(aq) + \text{CN}^-(aq)$		
Initial concentration (M)	0.15	0	0
Change (M)	$-x$	$+x$	$+x$
Equilibrium concentration (M)	$0.15 - x$	x	x

Approximation Example



$$K_c = \frac{(x)(x)}{0.150 - x} \approx \frac{x^2}{0.150}$$

$$x = \sqrt{0.150K_c} = \sqrt{(0.150)(4.9 \times 10^{-10})} = 8.6 \times 10^{-6} \text{ M}$$

$$[\text{HCN}] = 0.150 - x = 0.150 - (8.6 \times 10^{-6}) = 0.14999 \text{ M} \approx 0.150 \text{ M}$$

$$[\text{H}^+] = [\text{CN}^-] = x = 8.6 \times 10^{-6} \text{ M}$$