EQUILIBRIUM CALCULATIONS

- We're often interested in figuring out what happens at equilibrium BEFORE we do an experiment!

- What's the problem? Initially, we know only ... INITIAL concentrations. Since these are NOT equilibrium concentrations, we cannot simply plug them into an equilbrium expression and solve.

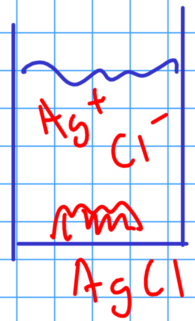
- So how do we find out what the concentrations are at equilibrium if we initially know NONE of them?

- To solve an equilibrium problem, write out the equilibrium constant expression. Then, try to RELATE ALL THE EQUILIBRIUM CONCENTRATIONS TO ONE ANOTHER using the chemical equation.

- It helps to assign a variable based on one of the substances in the reaction, then write the concentrations of the other substances based on that variable. How to do this? Take a look at the following examples...

EXAMPLE: Calculate the grams per liter of silver(i) chloride (AgCl) in a solution that is at equilibrium with solid AgCl.

$$AgCl(s) \rightleftharpoons Ag^+(aq) + Cl^-(aq) \; ; \; K_c = 1.8 \times 10^{-10}$$



$$K_c = [Ag^+][Cl^-] = 1.8 \times 10^{-10}$$

Assign a VARIABLE, x, to be equal to the change in silver concentration...

	Initial	Δ	Equilibrium
$[Ag^+]$	0	$+x$	x
$[Cl^-]$	0	$+x$	x

Since the concentrations of silver and chloride are RELATED, we can solve this problem!

$$[Ag^+][Cl^-] = 1.8 \times 10^{-10}$$

$$(x)(x) = 1.8 \times 10^{-10}$$

$$x^2 = 1.8 \times 10^{-10}$$

Take the quare root. Keep only the positive root.

$$x = 1.34 \times 10^{-5}\ \underline{M} = [Ag^+] = [Cl^-]$$

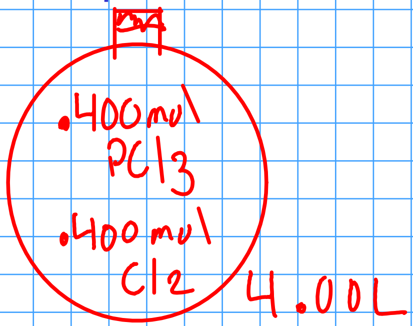
$$[AgCl] = 1.34 \times 10^{-5}\ \underline{M} \times 143.32 \frac{g}{mol} = \boxed{0.0019\ g/L}$$

(in solution)

Or, 1.9 mg/L (1.9 ppm)

$$PCl_3(g) + Cl_2(g) \rightleftharpoons PCl_5(g) \quad K_c = 49$$

If you add 0.400 moles of each reactant to a 4.00 L reaction vessel, what is the composition of the equilibrium mixture?



Initial conditions

$$K_c = \frac{[PCl_5]}{[PCl_3][Cl_2]} = 49$$

... we need to find these equilibrium concentrations!

	Initial	Δ	Equilibrium
$[PCl_5]$	0	$+x$	x
$[Cl_2]$	$\frac{.400\ mol}{4.00\ L} = .100$	$-x$	$0.100 - x$
$[PCl_3]$	$\frac{.400\ mol}{4.00\ L} = .100$	$-x$	$0.100 - x$

$$\frac{[PCl_5]}{[PCl_3][Cl_2]} = 49 = \frac{x}{(.100 - x)(.100 - x)}$$

We need to solve this expression for x!

We'd like to rearrange the equation to get x by itself ... Start by getting x out of the deniminator!

$$49 = \frac{x}{(.100 - x)(.100 - x)}$$

$$\downarrow$$

$$49(.100 - x)^2 = x$$

$$(a-b)^2 = a^2 - 2ab + b^2$$

$$49(0.0100 - .200x + x^2) = x$$

$$0.49 - 9.8x + 49x^2 = x$$

$$49x^2 + -10.8x + 0.49 = 0$$

$a = 49 \quad b = -10.8 \quad c = 0.49$

This is a QUADRATIC equation, which we can solve with the QUADRATIC FORMULA:

$$\boxed{\begin{gathered} ax^2 + bx + c = 0 \\ x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \end{gathered}}$$

Each quadratic has TWO solutions, but only ONE of these solutions is CHEMICALLY correct!

$$x = \frac{10.8 \pm \sqrt{(-10.8)^2 - 4(49)(0.49)}}{2(49)} = \frac{10.8 + \sqrt{20.6}}{98} \text{ OR } \frac{10.8 - \sqrt{20.6}}{98}$$

$$= \cancel{0.167} \text{ OR } 0.0639$$

Which one of these roots is the correct one?

This value gives us a negative concentration for both phosphorus trichloride AND for chlorine. That's physically impossible!

$$x = 0.0639\ \underline{M}$$

	Initial	Δ	Equilibrium
$[PCl_5]$	0	$+x$	x
$[Cl_2]$	$\frac{.400\text{ mol}}{4.00\text{ L}} = .100$	$-x$	$0.100 - x$
$[PCl_3]$	$\frac{.400\text{ mol}}{4.00\text{ L}} = .100$	$-x$	$0.100 - x$

Now, plug x in to find the concentrations of all species at equilibrium.

$x = 0.0639\ \underline{M}$

$[PCl_5] = x = 0.0639\ \underline{M} \times 4.00\text{ L} = .256\text{ mol } PCl_5$

$[Cl_2] = 0.100 - x = 0.0361\ \underline{M} \times 4.00\text{ L} = .144\text{ mol } Cl_2$

$[PCl_3] = 0.100 - x = 0.0361\ \underline{M} \times 4.00\text{ L} = .144\text{ mol } PCl_3$

Concentrations at equilibrium

Number of moles in reaction vessel at equilibrium