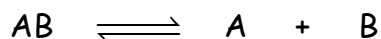


## Developing a Problem Solving Strategy for Chemical Equilibrium Problems

1. A balanced chemical reaction is needed.
2. Write an equilibrium constant expression in terms of the reaction.
3. Set-up the **ICE** chart as illustrated below using molar concentrations:



**I**nitial:

**C**hange:

**E**quilibrium:

4. Place any initial concentrations given into the **ICE** chart. Assume that all other concentrations in the reaction not given are zero.
  5. Consider the changes as the reaction shifts from the initial state towards equilibrium. Any initial zero concentrations must become an unknown value, "x", and all the change values must be in terms of "x", remember reaction stoichiometry and the signs of the changes ("+" if produced in the shift and any zero value must be produced, while "-" if consumed or reacted during the shift).
  6. Add the initial values and the change to get the equilibrium values.
  7. Substitute the equilibrium values in the equilibrium constant expression. Solve for the unknown value, x, and the equilibrium concentrations.
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Here is an example. A chemist has a container of  $A_2$  and  $B_2$  and they react as given below.



If 1.0 mole  $A_2$  and 1.0 mole  $B_2$  are placed in a 2.0 L container, what are the equilibrium concentrations of  $A_2$ ,  $B_2$ , and  $AB$ ? First find initial concentrations!

	$A_2$	+	$B_2$	$\rightleftharpoons$	$2 AB$	$K = (AB)^2 / (A_2)(B_2)$
<b>I</b> nitial:	0.50M		0.50M		0	
<b>C</b> hange:	$-\frac{1}{2} x$		$-\frac{1}{2} x$		$+ x$	(This <b>MUST</b> obey stoichiometry!)
<b>E</b> quilibrium:	$0.50M - \frac{1}{2} x$		$0.50M - \frac{1}{2} x$		$x$	

Place the equilibrium values into the equilibrium constant expression and solve for the value of x. Calculate the equilibrium concentrations of  $A_2$ ,  $B_2$ , and  $AB$ . Try it!

Try doing the math first and getting answers. The full solution is on the next page.

$$K = \frac{(AB)^2}{(A_2)(B_2)} = \frac{x^2}{(0.50 - \frac{1}{2}x)^2} = 9.0$$

you could solve this quadratic equation (see last page)

or in this case,

take the square root of both sides of the equation

$$\sqrt{\frac{x^2}{(0.50 - \frac{1}{2}x)^2}} = \sqrt{9.0}$$

$$\frac{x}{(0.50 - \frac{1}{2}x)} = 3.0$$

rearrange and solve for x

$$x = 3.0(0.50 - \frac{1}{2}x) = 1.5 - 1.5x$$

$$2.5x = 1.5$$

$$x = \frac{1.5}{2.5} = 0.60$$

so (AB) = x = 0.60 M and

$$(A_2) = (B_2) = 0.50 - \frac{1}{2}(0.60) = 0.20 \text{ M}$$

$$\text{as a check: } K = \frac{(0.60)^2}{(0.20)^2} = 9.0$$

Suppose you had a container that was 1.0 M in A (g) and it underwent the following reaction. Find the equilibrium concentrations of A<sub>2</sub> and A. Follow the steps outlined above!!!!



Initial:

Change:

Equilibrium:

(This MUST obey stoichiometry!)

Try to solve this problem before you view the solution. The full solution is on the next page.

Here is the full solution and it requires using the quadratic formula:

	$2 A$	$\rightleftharpoons$	$A_2$	$K = 4.0$ at $50^\circ\text{C}$	$K = (A_2)/(A)^2$
Initial:	1.0 M		0		
Change:	-2x		+ x		
Equilibrium:	1.0 - 2x		x		

$$K = \frac{(A_2)}{(A)^2} = \frac{x}{(1.0 - 2x)^2} = 4.0$$

$$x = 4.0 (1.0 - 2x)^2 = 4.0 (1.0 - 4x + 4x^2)$$

$$x = 4.0 - 16x + 16x^2$$

$$0 = 4.0 - 17x + 16x^2 = 16x^2 - 17x + 4.0$$

solve for x using the quadratic formula

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \frac{-(-17) \pm \sqrt{(-17)^2 - 4(16)(4.0)}}{2(16)}$$

$$= \frac{17 \pm \sqrt{289 - 256}}{32}$$

$$x_1 = \frac{17 + 5.7}{32} = 0.71 \quad [\text{max for } x = 0.5 \text{ for reaction to go to completion (LCM)}]$$

$$x_2 = \frac{17 - 5.7}{32} = 0.35 = (A_2) \quad \text{answer !!!!}$$

$$\text{as a check: } K = \frac{(A_2)}{(A)^2} = \frac{0.35}{(1.0 - 2(0.35))^2} = \frac{0.35}{(0.30)^2} = \frac{0.35}{0.090} = 3.9$$

which is very close to 4.0 considering only 2SF and rounding error

For more, see the general chemistry site at Purdue-

<http://www.chem.purdue.edu/gchelp/howtosolveit/Equilibrium/ICEchart.htm>

[http://www.chem.purdue.edu/gchelp/howtosolveit/Equilibrium/Calculating\\_Equilibrium\\_Constants.htm](http://www.chem.purdue.edu/gchelp/howtosolveit/Equilibrium/Calculating_Equilibrium_Constants.htm)

... or read the textbook for the course!!!!

If you grasp the use of the **ICE** chart now, it makes the upcoming acid-base equilibria easier to comprehend!

General comments about solving quadratic equations in equilibrium problems:

rearrange to equal zero

$$ax^2 + bx + c = 0$$

then substitute into the quadratic formula

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

always get two roots or solutions:  $x_1$  and  $x_2$

we always deal with real numbers, so

$$\sqrt{b^2 - 4ac} \geq 0$$

if negative, check your algebra!!!

$x_1$	$x_2$	What works?
+	+	Larger value of two will defy LCM!!! Use the smaller value.
+	-	Can't have negative concentrations!!! Use the positive value!!
-	-	Can't have both as negative concentrations!!! Check your algebra!!!

Make solving quadratic equations easy - for all the choices below, you must arrange the equation to set it equal to zero (do the algebra!) and have the values of a, b, and c ready to plug-in:

1. get a program for your TI-83/84 graphing calculator - see your instructor
2. use the quadratic solver in Excel available at:  
[http://academic.pgcc.edu/~ssinex/quad\\_behavior.xls](http://academic.pgcc.edu/~ssinex/quad_behavior.xls)  
(There is a link on the CHM 102 webpage as well.)
3. use the Java applet available at:  
<http://www.math.com/students/calculators/source/quadratic.htm>