you-try-it-05.xlsx
Step-by-Step Guide
ver. 7/26/2016

Abstract

This document provides step-by-step instructions for the Excel workbook you-try-it-05.xlsx (saved from Excel 2010). The worksheets contain data for practice exercises keyed to Chapter 5 of:

> *Basics of Analytical Chemistry and Chemical Equilibria* by Brian M. Tissue
> (John Wiley: New York, 2013).

General Advice

It is often useful to work out the first exercise of each worksheet on paper. After obtaining a result, compare your result to the answer in the worksheet. Next try writing formulas to do the calculation(s). If you do not get the same answer, try writing formulas stepwise and check intermediate steps to error check your work. Try to write formulas to be general so that you can copy them to use for multiple cases.

Version History

5/26/2009	First posting.
9/28/2009	Minor errors and formatting corrected.
7/26/2016	Formatting revisions.

For updates visit the text support website:

http://www.achem.org
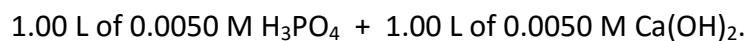
5.1 neutralization

This worksheet contains a table with pairs of solutions. One solution is of a strong acid and the other is of a strong base. The exercise is to determine the limiting reagent and the resulting $p[H_3O^+]$ when the two solutions are mixed.

Concepts	Concept Synopsis
stoichiometry	The stoichiometry of strong acids and strong bases determines how many H^+ or OH^- are available from each.
neutralization	H^+ will react with OH^- to form H_2O. "Excess" H^+ and OH^- will not exist together in solution, If there is an excess of either H^+ or OH^-, the concentration of the other ion is controlled by the K_w equilibrium.
limiting reagent	In neutralization reactions the number of moles of H^+ will react with the number of moles of OH^- until one or both are neutralized completely.

1. Determine if the acid or the base is the limiting reagent for each case.
    Optional: Write a formula to determine the limiting reagent.

2. Determine if the resulting solution will be acidic, basic, or neutral.

I will complete questions 1 and 2 together, illustrating the calculations with case 6:
    1.00 L of 0.0050 M H_3PO_4 + 1.00 L of 0.0050 M $Ca(OH)_2$.

First determine the number of moles of H^+ in the acid solution and the number of moles of OH^- in the base solution:
    (1.00 L)(0.0050 mol/L H_3PO_4)(3 mol H^+/1 mol H_3PO_4) = 0.0150 mol H^+
    (1.00 L)(0.0050 mol/L $Ca(OH)_2$)(2 mol OH^-/1 mol $Ca(OH)_2$) = 0.0100 mol OH^-

In looking at this result we can see that the base solution will be the limiting reagent. On mixing the two solutions, all of the OH^- will be neutralized and some amount of H^+ will remain, leading to an acidic solution.

To do this calculation in the worksheet, we need the number of moles of H^+ or OH^- for each acid and base. I copy the information in Table 5.1.A to a new location. I copy the case 6 information to rows 40 and 41, adding the stoichiometric factors:

	A	B	C	D	E	F	G	H	I	J
38								limiting	resulting	
39		case	vol (L)	conc (M)		# H or OH	mol	reagent	solution	pH
40		6	1.00	0.0050	H_3PO_4	3				
41			1.00	0.0050	$Ca(OH)_2$	2				

Now I have the information that I need for the calculation shown above. In cells G40 and G41 I type:

    =C40*D40*F40
    =C41*D41*F41

I get the same result as above. I type in the results for 'limiting reagent' and 'resulting solution' and add units, sample formulas and more formatting to produce something like:

	A	B	C	D	E	F	G	H	I	J
37										
38								limiting	resulting	
39		case	vol (L)	conc (M)		# H or OH	mol	reagent	solution	pH
40		6	1.00	0.0050	H_3PO_4	3	0.015	base	acidic	
41			1.00	0.0050	$Ca(OH)_2$	2	0.010			
42			L	mol/L			mol			
43							=C40*D40*F40			

For the optional part of the question, I can write an Excel formula to determine the limiting reagent using an IF statement to compare the number of moles of acid and base. In cell H40 I type:

    =IF($G40>$G41,"base","acid")

The IF function checks if the listed logic condition is true and then returns the first option, the text "base". If the condition is not true, the function returns the second option, the text "acid".

This formula does not work correctly if the number of moles of acid and base are equal. For that possibility we can nest two IF functions to first test if the numbers of moles are equal. If the condition is not true, then the second option is the nested IF function as above.

=IF($G40=$G41,"both",IF($G40>$G41,"base","acid"))

The result will look the same as typed in the figure above. I can use the same type of nested IF statements to specify if the solution is acidic, basic, or neutral. The only changes that I make in the formula is for the responses returned by the IF functions:

=IF($G40=$G41,"neutral",IF($G40>$G41,"acidic","basic"))

The result is again the same as seen in column I in the figure above.

3. Write formulas to calculate the $p[H_3O^+]$ of the solution when the acid and base are mixed.

The calculation is $p[H_3O^+]$ = $-\log[H_3O^+]$. We have three possible cases when our solutions are mixed:

- excess H_3O^+, $p[H_3O^+]$ = $-\log[H_3O^+]$
- excess OH^-, $p[H_3O^+]$ = 14.00 $-(-\log[OH^-])$ = 14.00 + $\log[OH^-]$
- H_3O^+ and OH^- neutralized completely, $p[H_3O^+]$ is approximately 7.

Again using case 6 as my example, the calculation for an acidic solution is:

$[H_3O^+]$ = (mol H_3O^+)/volume

= (0.0150 mol H^+ − 0.0100 mol OH^-)/(1.00 L + 1.00 L)

= (0.0050 mol H^+)/(2.00 L)

= (0.0050 mol H^+)/(2.00 L) = 0.0025 M

$p[H_3O^+]$ = $-\log[H_3O^+]$ = $-\log(0.0025$ M) = 2.60

We can enter a different formula for each case, depending if the resulting solution is neutral, acid, or basic. I will use IF functions to test for these cases to select the appropriate formula. The first IF function tests if the H_3O^+ and OH^- neutralized completely:

=IF($I40="neutral","~7", nested IF function)

If this condition is not met, the 'nested IF function' uses a different formula for either excess H_3O^+ or excess OH^-.

The Excel formula in the nested IF function is:

IF($I40="acidic",-LOG(($G40-$G41)/($C40+$C41)),14+LOG(($G41-$G40)/($C40+$C41)))

Overall, in cell J40 I type:

=IF($I40="neutral","~7",   IF($I40="acidic",-LOG(($G40-$G41)/($C40+$C41)),14+LOG(($G41-$G40)/($ C40+$C41))))

I can copy this formula to the other cases, and my overall results appear like the following figure:

	A	B	C	D	E	F	G	H	I	J
27										
28								limiting	resulting	
29		case	vol (L)	conc (M)		# H or OH	mol	reagent	solution	p[H_3O^+]
30		1	1.00	0.0070	HCl	1	0.007	base	acidic	3.00
31			1.00	0.0050	KOH	1	0.005			
32		2	1.00	0.0050	HNO_3	1	0.005	acid	basic	11.00
33			1.00	0.0070	NaOH	1	0.007			
34		3	1.00	0.0050	H_2SO_4	2	0.010	base	acidic	2.60
35			1.00	0.0050	LiOH	1	0.005			
36		4	1.00	0.0050	H_2SO_4	2	0.010	both	neutral	~7
37			1.00	0.0050	$Ca(OH)_2$	2	0.010			
38		5	1.00	0.0050	$HClO_4$	1	0.005	acid	basic	11.40
39			1.00	0.0050	$Ca(OH)_2$	2	0.010			
40		6	1.00	0.0050	H_3PO_4	3	0.015	base	acidic	2.60
41			1.00	0.0050	$Ca(OH)_2$	2	0.010			
42										
43			L	mol/L			mol			
44							=C30*D30*F30			

5.2 amphiprotic-salts

This worksheet contains a table listing different salts. The key aspect of the exercise is to correctly identify the nature of the cation and the anion of each salt. Strong electrolytes do not react with water and do not directly affect the pH of a solution when dissolved. Ions that are not strong electrolytes will be weak acids or weak bases and will affect the pH of water. A salt that consists of both a weak acid and a weak base is called amphiprotic. To determine if the resulting solution is acidic or basic, compare the K_a and K_b of the constituent ions. If $K_a > K_b$ the solution will be acidic and if $K_b > K_a$ the solution will be basic.

Concepts	Concept Synopsis
salts	A soluble salt is an ionic compound that dissolves in water. The effect on a solution depends on the nature of the constituent ions.
weak acid equilibrium	A weak acid will partly react with water to form some amount of H_3O^+ and the conjugate base.
weak base equilibrium	A weak base will partly react with water to form some amount of OH^- and the conjugate acid.
K_w	We can determine the K_b of a weak base from the K_a of its conjugate acid using $K_w = K_a \times K_b$.

1. Look up K_a for the weak acid cations and the conjugate acids of the weak base anions.

The figure below shows one way to organize the data. The K_a values are formatted in scientific notation. I have entered 0.0 for the strong electrolytes to be compatible with IF functions that I will use later. I place the K_a values of the conjugate acid in column H so that I can place K_b values in column G.

	A	B	C	D	E	F	G	H	I
14						$K_w =$	1.01E-14		
15									
16		case		salt		cation K_a	anion K_b	K_a of conj. acid	result
17		1		KNO_3		0.00E+00		0.00E+00	
18		2		NH_4Cl		5.68E-10		0.00E+00	
19		3		CH_3COONa		0.00E+00		1.75E-05	
20		4		$Cu(CH_3COO)_2$		4.57E-08		1.75E-05	
21		5		NH_4F		5.68E-10		6.31E-04	
22		6		CH_3COONH_4		5.68E-10		1.75E-05	

2. Calculate K_b values for the weak base anions.
   Determine if the resulting solution will be acidic, basic, or neutral when the salt is dissolved in water.

The value of K_w is typed in cell G14. Using the K_a values for the conjugate acids of the anions in column H and the relation:

$$K_w = K_a \times K_b$$

we can determine K_b for each anion. For case 1 I type in cell G17:

=$G$14/H17

This gives me an error message. I can ignore the error and copy the formula down the column. I can now compare the K_a and K_b values and type acidic, basic, or neutral for each case. Our rules for determining the acidity of a solution containing both an acidic and a basic species are:

- If K_a of the cation is greater than K_b of the anion then the solution will be acidic.
- If K_b of the anion is greater than K_a of the cation then the solution will be basic.
- If $K_a = K_b$, as for two strong electrolytes, the solution will be neutral.

To write a more general formula, I use an IF function to test if the value in column H is zero. If there is a zero, then the IF function will return a 0.0 and if not it performs the calculation. The revised formula in cell G17 is:

=IF(H17=0,0,$G$14/H17)

The error message for case 1 is now replaced by 0.0. Copy this formula down the column and the formula will return either a 0.0 or the calculated value of K_b. Now to an-

swer the question of solution acidity, I use nested IF functions to test if $K_a = K_b$ and then if $K_a > K_b$. The formula that I use in cell I17 is:

=IF(F17=G17,"neutral",IF(F17>G17,"acidic","basic"))

Copying this formula to the other cells in column I gives me a result for each case. The final results are summarized in the figure below. A limitation of a worksheet formula is that it gives me an answer but does no thinking. On inspecting the K_a and K_b values, I see that they are almost equal in case 6. I make a note since I expect this solution to be nearly neutral.

A	B	C	D	E	F	G	H	I	J
14					$K_w =$	1.01E-14			
15									
16	case		salt		cation K_a	anion K_b	K_a of conj. acid	result	
17	1		KNO_3		0.00E+00	0.00E+00	0.00E+00	neutral	
18	2		NH_4Cl		5.68E-10	0.00E+00	0.00E+00	acidic	
19	3		CH_3COONa		0.00E+00	5.77E-10	1.75E-05	basic	
20	4		$Cu(CH_3COO)_2$		4.57E-08	5.77E-10	1.75E-05	acidic	
21	5		NH_4F		5.68E-10	1.60E-11	6.31E-04	acidic	
22	6		CH_3COONH_4		5.68E-10	5.77E-10	1.75E-05	basic	(near neutral)

5.3 acidity

This worksheet contains two tables: Table 5.3.A with two different solutions of acids and Table 5.3.B with two different solutions of bases. The first step is to identify strong versus weak acids and bases. Knowing the nature of each acid or base, you can then determine their relative acidity or basicity.

Concepts	Concept Synopsis
strong vs weak acids	A strong acid consists of one or more H^+ with a strong electrolyte as its anion. Anything else that can provide H^+ to solution is a weak acid.
strong vs weak bases	A strong base consists of one or more OH^- with a strong electrolyte as its cation. Anything else that can produce OH^- in solution is a weak base.
relative acidity	The extent to which a weak acid (or weak base) reacts with water is given by its K_a (or K_b) constant.

1. Predict which solution for each case in Table 5.3.A will be most acidic, i.e., will have the lowest pH.
   Calculate $p[H_3O^+]$ as needed for weak acids using $[H_3O^+] \approx sqrt(c_{HA}*K_a)$.

Looking at the acids in Table 5.3.A, HCl and HNO_3 are strong acids and the rest are weak acids. For case 1, the concentrations of the two acids are equal, but since solution 1 contains a strong acid and solution 2 contains a weak acid, we know that solution 1 will be more acidic. The strong acid dissociates completely, but the weak acid dissociates only partially.

For case 2 we again have a strong acid and a weak acid, but the concentrations are different and it is not obvious which solution will be the most acidic. We will calculate the $p[H_3O^+]$ for each solution to compare them. For the strong acid (solution 1), $[H_3O^+] = c_{HA}$ and $p[H_3O^+] = -\log[H_3O^+]$. The Excel formula that I type in cell E26 is:

    = -log(C26)

For the weak acid (solution 2), I calculate $[H_3O^+]$ using the approximation $[H_3O^+] \approx sqrt(c_{HA}*K_a)$. K_a values for the weak acids are in cells E17:E20. The Excel formula that I type in cell H26 is:

    = -LOG(SQRT(F26*$E$17))

Now comparing $p[H_3O^+]$ for these two solutions we see that solution 1 is more acidic. I copy the formulas in cells E26 and H26 to the row above, and the results are in the next figure:

	A	B	C	D	E	F	G	H	I
16				weak acid	K_a		weak base	K_b	
17				CH_3COOH	1.75E-05		NH_3	1.78E-05	
18				$CHCl_2COOH$	4.47E-02		$C_3H_4N_2$	1.02E-07	
19				$HClO$	2.90E-08		(imidazole)		
20				NH_4Cl	5.68E-10				
21									
22		Table 5.3.A							
23				acid solution 1			acid solution 2		most
24		case	conc (M)	acid	$p[H_3O^+]$	conc (M)	acid	$p[H_3O^+]$	acidic
25		1	0.0050	HCl	2.30	0.0050	CH_3COOH	3.53	soln 1
26		2	0.0050	HNO_3	2.30	0.0500	CH_3COOH	3.03	soln 1
27		3	0.0050	CH_3COOH		0.0050	$CHCl_2COOH$		
28		4	0.0050	CH_3COOH		0.0050	$HClO$		
29		5	0.0050	CH_3COOH		0.0500	NH_4Cl		

Cases 3-5 are pairs of weak acids. Before starting a calculation, try to answer which one is more acidic based on reasoning or estimating. For cases 3 and 4 the formal concentrations of the weak acids are the same. In these cases the one with the larger K_a will produce the more acidic solution. For case 3 this is solution 2, $CHCl_3COOH$, and for case 4 the stronger is solution 1, CH_3COOH. For case 5 the concentrations are different and it is again not obvious which solution will be more acidic. I use the same expression as above, changing the formula for the K_a specific weak acid. In cells E29 and H29 I enter:

    = -LOG(SQRT(C26*$E$17))
    = -LOG(SQRT(F26*$E$20))

I enter these types of formulas for the other cells that I have already answered for completeness. The overall results are in the next figure.

	A	B	C	D	E	F	G	H	I
22		Table 5.3.A							
23				acid solution 1			acid solution 2		most
24		case	conc (M)	acid	$p[H_3O^+]$	conc (M)	acid	$p[H_3O^+]$	acidic
25		1	0.0050	HCl	2.30	0.0050	CH_3COOH	3.53	soln 1
26		2	0.0050	HNO_3	2.30	0.0500	CH_3COOH	3.03	soln 1
27		3	0.0050	CH_3COOH	3.53	0.0050	$CHCl_2COOH$	1.83	soln 2
28		4	0.0050	CH_3COOH	3.53	0.0050	$HClO$	4.92	soln 1
29		5	0.0050	CH_3COOH	3.53	0.0500	NH_4Cl	5.27	soln 1

2. Predict which solution for each case in Table 5.3.B will be most basic, i.e., will have the highest pH.
No calculations are necessary.

For each pair of the base solutions we can reason which one will be the most basic. Case 1 compares two strong bases. They are present at the same formal concentration, but solution 2 contains two OH^- per formula unit. Due to the higher concentration of OH^-, solution 2 will be more basic.

Case 2 compares a weak base, solution 1, to a strong base. Since they have equal formal concentrations, we know the strong base solution will be more basic.

Case 3 compares two weak bases. Since they have equal formal concentrations, we know the weak base with the larger K_b will produce the be more basic solution.

Although not necessary, I include in the results calculations of $p[H_3O^+]$. The formulas are similar to the acids, but finding $p[OH^-]$. I use the relationship $14.00 = p[H_3O^+] + p[OH^-]$ to convert the result to $p[H_3O^+]$. My final answers are shown in the next figure.

	A	B	C	D	E	F	G	H	I
32		Table 5.3.B							
33				base solution 1			base solution 2		most
34		case	conc (M)	base	$p[H_3O^+]$	conc (M)	base	$p[H_3O^+]$	basic
35		1	0.0010	LiOH	11.00	0.0010	$Ca(OH)_2$	11.30	soln 2
36		2	0.0050	NH_3	10.47	0.0050	NaOH	11.70	soln 2
37		3	0.0050	NH_3	10.47	0.0050	$C_3H_4N_2$	9.35	soln 1

5.4 ionic-strength

This worksheet contains a table of solutions to calculate ionic strength. For two cases the activity coefficients are calculated for the reactants and products of the equilibrium reaction.

Concepts	Concept Synopsis
formal concentration	The species concentration before equilibrium is established.
ionic strength	A measure of the ionic charge in a solution: $I_c = 0.5\sum c_i z_i^2$
activity coefficients	The correction factors, γ_i, to find formal equilibrium constants, K', from tabulated thermodynamic equilibrium constants, K.

1. Calculate the ionic strength, I_c, for each solution in Table 5.4.A.
   The listed concentrations are formal concentrations before any reaction occurs.
   For cases 1-7 you may assume that reaction with water does not change I_c.
   For cases 5, 6, and 8, determine the ion concentrations after reaction and then calculate I_c.

To facilitate writing formulas to find I_c, I copy information from Table 5.4.A to a new location. I need the concentration and charge of each ion. The figure below shows one approach (showing cases 1 and 2).

	A	B	C	D	E	F	G	H	I	J	K	L
16		Table 5.4.A										
17		case	conc (M)	salt	conc (M)	salt		Notes				
18		1	0.0100	$CaCl_2$				Ca^{2+} is a borderline strong electrolyte				
19		2	0.0100	Na_3PO_4				PO_4^{3-} is a weak base				
20		3	0.0100	Na_2HPO_4				HPO_4^{2-} is amphiprotic				
21		4	0.0100	NaCl	0.0100	$CaCl_2$		Ca^{2+} is a borderline strong electrolyte				
22		5	0.0200	NaCl	0.0100	$Ba(NO_3)_2$		a precipitation reaction occurs				
23		6	0.0500	HNO_3	0.0100	$Ca(OH)_2$		a neutralization reaction occurs				
24		7	0.0500	NH_4Cl				NH_4^+ is a weak acid, $K_a = 5.675E\text{-}10$				
25		8	0.0500	NH_3				NH_3 is a weak base, $K_b = 1.780E\text{-}5$				
26												
27												
28		case	conc (M)	cation	charge	conc (M)	anion	charge	conc (M)	ion	charge	I_c (M)
29		1	0.0100	Ca^{2+}	2	0.0200	Cl^-	-1				
30		2	0.0300	Na^+	1	0.0100	PO_4^{3-}	-3				

I've typed the ions in columns D and G with their respective charges in columns E and H. I get the concentrations from column C in Table 5.4.A. The ion concentrations are de-

pendent on stoichiometry, and I've entered =C18 and =C18*2 in cells C29 and F29, respectively, for case 1. I fill out this new table for all of the cases. Columns I:K are only filled for the cases that have three ions in solution.

Calculate ionic strength using the expression:
$$I_c = 0.5 \sum c_i z_i^2$$
where c_i is the concentration of each ion and z_i is the charge of each ion.

Using case 1 as an example, the Excel formula that I type in cell L29 is:
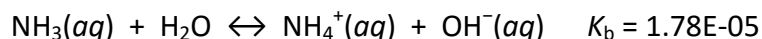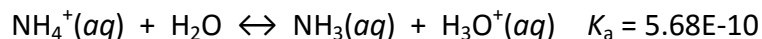   =0.5*(C29*E29^2+F29*H29^2+I29*K29^2)

I've included columns I and K in this formula, which I do not need for case 1. I include them so that I can copy the formula down the column and have it correct for all of the cases. I copy this formula into cells L30:L36 to calculate the ionic strength for each case, giving the results in the next figure.

	A	B	C	D	E	F	G	H	I	J	K	L
27												
28		case	conc (M)	cation	charge	conc (M)	anion	charge	conc (M)	ion	charge	I_c (M)
29		1	0.0100	Ca^{2+}	2	0.0200	Cl^-	-1				0.030
30		2	0.0300	Na^+	1	0.0100	PO_4^{3-}	-3				0.060
31		3	0.0200	Na^+	1	0.0100	HPO_4^{2-}	-2				0.030
32		4	0.0100	Na^+	1	0.0300	Cl^-	-1	0.0100	Ca^{2+}	2	0.040
33		5	0.0200	Na^+	1	0.0200	NO_3^-	-1				0.020
34		6	0.0300	H^+	1	0.0500	NO_3^-	-1	0.0100	Ca^{2+}	2	0.060
35		7	0.0500	NH_4^+	1	0.0500	Cl^-	-1				0.050
36		8	0.0000	NH_4^+	1	0.0000	OH^-	-1				0.0000

The I_c formula is quite straightforward. The places where errors occur are in entering the concentrations and charges correctly. If any values of I_c appear unusual to you, double check the entries in the table. Note that in case 5 that the concentrations of Ba^{2+} and Cl^- are not included due the precipitation reaction. Similarly, in case 6 the concentration of OH^- is not included since it is neutralized by the acid.

The equilibria in cases 7 and 8 are:

$$NH_4^+(aq) + H_2O \leftrightarrow NH_3(aq) + H_3O^+(aq) \quad K_a = 5.68E\text{-}10$$
$$NH_3(aq) + H_2O \leftrightarrow NH_4^+(aq) + OH^-(aq) \quad K_b = 1.78E\text{-}05$$

I type the K_a and K_b values in cells I41 and I 42, respectively, to be able to reference them in formulas.

Given I_c, we can calculate activity coefficients using the Debye-Hückel equation. This formula is already in activity-coefficients.xlsx, so open that spreadsheet and find the activity coefficients for the ions involved in the equilibria in cases 7 and 8. I copy the values to this spreadsheet:

▲ A	B	C	D	E	F	G	H	I
38								
39	activity coefficients copied from activity-coefficients.xlsx							
40	case	NH_4^+	OH^-	H^+		Thermodynamic K values		
41	7	0.801		0.854		NH_4^+	$K_a =$	5.68E-10
42	8	0.966	0.967			NH_3	$K_b =$	1.78E-05

Rearranging the expressions for K_a and K_b and replacing activity with concentration and activity coefficients (see example 5.17 in the text), we find:

$$K_a' = (K_a)(\gamma_{NH4}) / \gamma_{H3O}$$
$$K_b' = K_b / (\gamma_{NH4})(\gamma_{OH})$$

The calculations are:

$$K_a' = \frac{5.68\times10^{-10}}{0.854} = 5.32\times10^{-10}$$

$$K_b' = \frac{1.78\times10^{-5}}{(0.966)(0.967)} = 1.91\times10^{-5}$$

In Excel, to find K_a' I type in cell I45:

=I41*C41/E41

To find K_b' I type in cell I46:

$\qquad$ =I42/(C42*D42)

The results are:

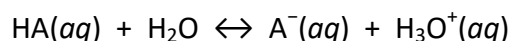| ◢	A	B	C	D	E	F	G	H	I
43									
44							Corrected K values		
45							NH_4^+	$K_a' =$	5.32E-10
46							NH_3	$K_b' =$	1.91E-05

5.5 equilibrium-calculation

This worksheet contains examples of weak acid and weak base solutions and asks to find p[H_3O^+] for each.

Concepts	Concept Synopsis
weak acid equilibrium calculation	Writing the correct K_a' expression for a weak acid and solving for [H_3O^+] and p[H_3O^+].
weak base equilibrium calculation	Writing the correct K_b' expression for a weak base and solving for [OH^-] and p[H_3O^+].

1. Write formulas to find [H_3O^+] and p[H_3O^+] for the weak acid solutions in Table 5.5.A. Use the approximation [H_3O^+] ≈ sqrt($c_{HA}*K_a$).
    Do the same for the weak bases in Table 5.5.B, solving for [OH^-] and converting to [H_3O^+].

A weak acid reacts with water to form the following equilibrium:

$$HA(aq) + H_2O \leftrightarrow A^-(aq) + H_3O^+(aq)$$

For a solution that is prepared from the weak acid with no addition of the conjugate base, [A^-] = [H_3O^+], and the equilibrium constant expression can be simplified as follows:

$$K_a' = \frac{[A^-][H_3O^+]}{[HA]} = \frac{[H_3O^+]^2}{c_{HA} - [H_3O^+]}$$

Neglecting [H_3O^+] compared to c_{HA} gives us the approximation: [H_3O^+] ≈ sqrt($c_{HA}\ K_a'$). This calculation is the same as we did in worksheet 5.3 for the weak acids. For case 1, I type in cells G18 and H18:

    =SQRT(C18*E18)   =-log(G18)

Copying these formulas down the next three rows gives the results in the next figure.

	A	B	C	D	E	F	G	H
15								
16		Table 5.5.A Weak Acids					approximate solution	
17		case	conc (M)	acid	K_a'		$[H_3O^+]$	$p[H_3O^+]$
18		1	0.0100	CH_3COOH	1.8E-05		4.24E-04	3.37
19		2	0.0010	CH_3COOH	1.8E-05		1.34E-04	3.87
20		3	0.0010	NH_4Cl	5.7E-10		7.55E-07	6.12
21		4	0.0100	$CHCl_2COOH$	5.7E-02		2.39E-02	1.62

The calculation for the weak bases is the same as above, although now solving for [OH⁻]. The equilibrium is:

$$B(aq) + H_2O \leftrightarrow HB^+(aq) + OH^-(aq)$$

My generic examples show the weak base, B, and the HA weak acid above, both being neutral. Weak acids and weak bases can be charged, with a corresponding change in the conjugate species.

For a solution that is prepared from the weak base with no addition of the conjugate acid, $[HB^+]$ = $[OH^-]$, and the equilibrium constant expression can be simplified as follows:

$$K_b' = \frac{[HB^+][OH^-]}{[B]} = \frac{[OH^-]^2}{c_B - [OH^-]}$$

Neglecting [OH⁻] compared to c_B gives us the approximation: $[OH^-] \approx sqrt(c_B\ K_b')$. For case 1 in Table 5.5.B, I type in cells G26 and H26:
        =SQRT(C26*E26)   =-log(G26)

The last step is then to convert p[OH⁻] to $p[H_3O^+]$ using $p[H_3O^+]$ + p[OH⁻] = 14.00. I type in cell I26:
        =14-H26

Copying these formulas to the next row gives the results in the next figure.

	A	B	C	D	E	F	G	H	I
23									
24		Table 5.5.B Weak Bases					approximate solution		
25		case	conc (M)	base	K_b'		[OH⁻]	p[OH⁻]	$p[H_3O^+]$
26		1	0.0010	NH_3	1.8E-05		1.34E-04	3.87	10.13
27		2	0.0010	NaClO	3.5E-07		1.87E-05	4.73	9.27

2. Write formulas to find $[H_3O^+]$ and $p[H_3O^+]$ for the weak acid solutions in Table 5.5.A. Use the quadratic equation and compare your results with the approximation in question 1.

When the approximation in question 1 is not valid, the equilibrium constant expression must be solved with the quadratic equation:

$$K_a' = \frac{[A^-][H_3O^+]}{[HA]} = \frac{[H_3O^+]^2}{c_{HA} - [H_3O^+]}$$

A quadratic equation of the form $ax^2+bx+c = 0$ will have two roots. We may ignore the negative root, it has no physical meaning. Rearranging the equilibrium constant expression gives:

$$[H_3O^+]^2 + (K_a')[H_3O^+] - (K_a')(c_{HA}) = 0$$

The expression in Excel format for the positive root is:
=(-b+SQRT (b^2-4*a*c))/(2*a)

In our case $a = 1$, $b = K_a'$, and $c = -(K_a')(c_{HA})$, so this formula simplifies to:
=(-b+ SQRT(b^2+4*c))/2

On replacing b and c with cell locations, for case 1 I type in cell I18:
=(-$E18+SQRT($E18^2+4*$C18*$E18))/2

I take the –log in column J, copy the formulas down the columns, and the final results are:

A	B	C	D	E	F	G	H	I	J
15									
16	Table 5.5.A Weak Acids					approximate solution		quadratic solution	
17	case	conc (M)	acid	K_a'		$[H_3O^+]$	$p[H_3O^+]$	$[H_3O^+]$	$p[H_3O^+]$
18	1	0.0100	CH₃COOH	1.8E-05		4.24E-04	3.37	4.15E-04	3.38
19	2	0.0010	CH₃COOH	1.8E-05		1.34E-04	3.87	1.25E-04	3.90
20	3	0.0010	NH₄Cl	5.7E-10		7.55E-07	6.12	7.55E-07	6.12
21	4	0.0100	CHCl₂COOH	5.7E-02		2.39E-02	1.62	8.68E-03	2.06

Looking at the results, we can see that there is not too much difference between the approximate and the quadratic equation solutions except for $CHCl_2COOH$. This acid is a

relatively strong weak acid, and $[H_3O^+]$ cannot be neglected compared to c_{HA}. For the case of CH_3COOH, the approximate result does get a little worse at lower concentration (case 2 compared to case 1).

I did not ask for quadratic solutions for the solutions of weak bases in Table 5.5.B. Given the K_b' values of these two weak bases, should I redo the calculation with the quadratic equation or do you think that the approximate results are accurate?