

**you-try-it-06.xlsx**

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For use with:

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

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Worksheets in this file

notes	This page with background information.
6.A Henderson-Hasselbalch	Henderson-Hasselbalch calculations as a function of concentration.
6.B polyprotic-acid	Predict the pH for each buffer system.
6.C polyprotic-buffer	Determine buffer preparation from listed starting materials.
6.D carbonic-acid	Predict the pH for each carbonate-containing system.

Background

Refer to Chapter 6 in the text for equations and explanations.

Each worksheet has instructions in the shaded box.

For step-by-step help see [you-try-it-06guide.pdf](#).

Tables of thermodynamic  $K_a$  values for weak acids are available in:

- Appendix C of the text.

- 'K<sub>a</sub> values' worksheet in [pH-calculation.xlsx](#).

(Use 'Copy' and 'Paste Values' to copy values to this worksheet.)

**You-Try-It 6.A Henderson-Hasselbalch Calculation for pH Buffer**

Table 6.A.1 lists a series of acid/base buffers.

1. Use the Henderson-Hasselbalch equation to predict the  $p[H_3O^+]$  for each buffer solution. You may do your calculations assuming that  $K_a' = K_a$ .
2. Calculate the difference in  $p[H_3O^+]$  between the Henderson-Hasselbalch and exact results. What factors affect the accuracy of the Henderson-Hasselbalch equation?

weak acid	$K_a$	$pK_a$
acetic acid	1.75E-05	4.757
chloroacetic acid	1.36E-03	2.866
dichloroacetic acid	4.47E-02	1.350

**Table 6.A.1**

case		$K_a'$	$c_{acid}$	$c_{base}$	H-H Eqn $p[H_3O^+]$	Exact $p[H_3O^+]$	Difference $p[H_3O^+]$
1	acetic acid	1.750E-05	1.000E-01	1.000E-01		4.757	
2	acetic acid	1.750E-05	1.000E-02	1.000E-02		4.758	
3	acetic acid	1.750E-05	1.000E-03	1.000E-03		4.772	
4	acetic acid	1.750E-05	1.000E-04	1.000E-04		4.874	
5	chloroacetic acid	1.360E-03	1.000E-01	1.000E-01		2.878	
6	chloroacetic acid	1.360E-03	1.000E-02	1.000E-02		2.962	
7	chloroacetic acid	1.360E-03	1.000E-03	1.000E-03		3.320	
8	chloroacetic acid	1.360E-03	1.000E-04	1.000E-04		4.056	
9	dichloroacetic acid	4.470E-02	1.000E-01	1.000E-01		1.582	
10	dichloroacetic acid	4.470E-02	1.000E-02	1.000E-02		2.142	
11	dichloroacetic acid	4.470E-02	1.000E-03	1.000E-03		3.019	
12	dichloroacetic acid	4.470E-02	1.000E-04	1.000E-04		4.002	

Do not overwrite formulas in these shaded cells.

$K_w$ : 1.01E-14

Exact pH calculation for an acid-base buffer (copied from pH-calculation.xlsx)

$a_1$	$a_2$	$a_3$	Q	R	$Q^3-R^2$	theta	$x_2$
1.000E-01	-1.75E-06	-1.768E-19	0.0011121	3.70857E-05	2.839E-16	0.0004543	1.749E-05
1.002E-02	-1.75E-07	-1.768E-19	1.121E-05	3.7524E-08	2.865E-20	0.0045111	1.744E-05
1.018E-03	-1.75E-08	-1.768E-19	1.209E-07	4.19834E-11	3.134E-24	0.0421438	1.692E-05
1.175E-04	-1.75001E-09	-1.768E-19	2.117E-09	9.43537E-14	5.9E-28	0.2519671	1.337E-05
1.014E-01	-0.000136	-1.374E-17	0.0011869	4.08663E-05	1.853E-12	0.0332944	1.324E-03
1.136E-02	-1.36E-05	-1.374E-17	1.887E-05	8.00458E-08	3.142E-16	0.217919	1.092E-03
2.360E-03	-1.36E-06	-1.374E-17	1.072E-06	1.02176E-09	1.885E-19	0.4018508	4.790E-04
1.460E-03	-1.36E-07	-1.374E-17	2.822E-07	1.48358E-10	4.582E-22	0.1432985	8.786E-05
1.447E-01	-0.00447	-4.515E-16	0.0038165	0.000220014	7.182E-09	0.3676643	2.616E-02
5.470E-02	-0.000447	-4.515E-16	0.0004815	1.01369E-05	8.844E-12	0.2853586	7.219E-03
4.570E-02	-4.47E-05	-4.515E-16	0.000247	3.87543E-06	4.195E-14	0.052799	9.580E-04
4.480E-02	-4.47E-06	-4.515E-16	0.0002245	3.36358E-06	3.746E-16	0.0057543	9.956E-05

**You-Try-It 6.B**                      **p[H<sub>3</sub>O<sup>+</sup>] of Polyprotic Acid Solutions**

Table 6.B.1 gives formal concentrations of polyprotic acids.

- Predict the p[H<sub>3</sub>O<sup>+</sup>] for each solution.  
You may do your calculations assuming that  $K_a' = K_a$ .  
You may use the Henderson-Hasselbalch equation for buffer solutions.

polyprotic acid	base form	acid formula	$K_a$	$pK_a$
phthalic acid	hydrogen phthalate	$C_6H_4(COOH)_2$	1.12E-03	2.950
hydrogen phthalate	phthalate ion	$C_8H_5O_4^-$	3.91E-06	5.408
phosphoric acid	dihydrogen phosphate	$H_3PO_4$	7.11E-03	2.148
dihydrogen phosphate	hydrogen phosphate	$H_2PO_4^-$	6.34E-08	7.198
hydrogen phosphate	phosphate ion	$HPO_4^{2-}$	4.79E-13	12.32

**Table 6.B.1**

case	
1	0.01 M phthalic acid
2	0.01 M sodium hydrogen phthalate
3	0.01 M disodium phthalate
4	0.03 M phosphoric acid, 0.01 M sodium dihydrogen phosphate
5	0.01 M disodium hydrogen phosphate
6	0.01 M sodium dihydrogen phosphate, 0.005 M disodium hydrogen phosphate

case	calc. type	$c_{HA}$	$c_{A^-}$	$K_a', K_b', \text{ or}$		$[H_3O^+]$	$[OH^-]$	$p[H_3O^+]$
				$pK_a'$	$pK_{a2}'$			
1								
2								
3								
4								
5								
6								

**You-Try-It 6.C****Preparing Polyprotic Buffers**

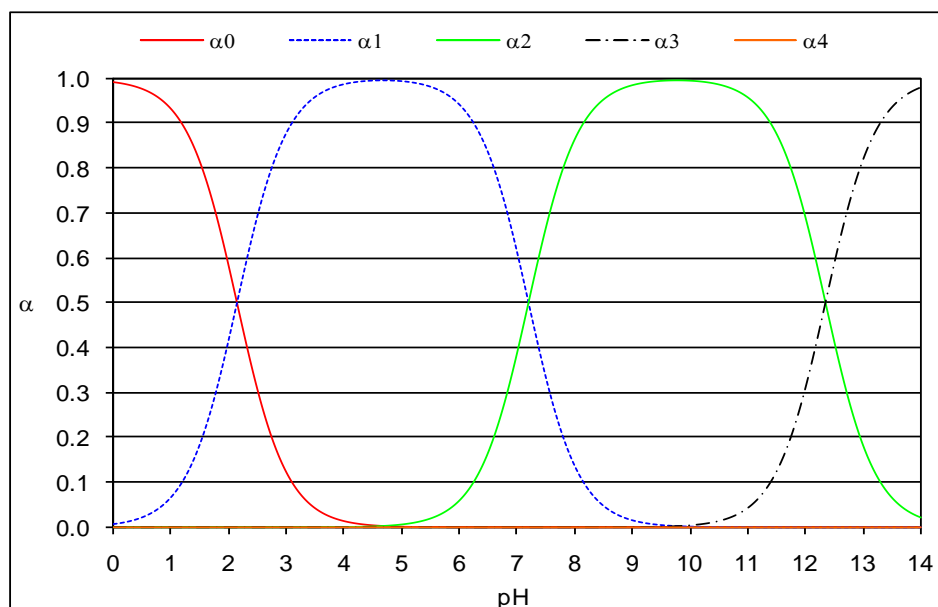
Table 6.C.1 gives starting materials to make the listed buffer solutions.  
You also have 0.5 M NaOH and 0.5 M HCl.

1. Give a procedure to prepare 1.0 L of the listed buffer from the starting material.  
You may do your calculations assuming that  $K_a' = K_a$ .  
You may use the Henderson-Hasselbalch equation for buffer calculations.

	formula	f.w. (g/mol)	$K_a$	$pK_a$
phosphoric acid	$H_3PO_4$	98.00	7.11E-03	2.148
sodium dihydrogen phosphate	$NaH_2PO_4$	119.98	6.34E-08	7.198
disodium hydrogen phosphate	$Na_2HPO_4$	141.96	4.79E-13	12.32
trisodium phosphate	$Na_3PO_4$	163.94		

**Table 6.C.1**

case	starting material	total $C_{\text{phosphate}}$	desired $p[H_3O^+]$
1	concentrated (14 M) phosphoric acid	0.1 M	7.4
2	0.5 L of 0.2 M sodium dihydrogen phosphate	0.1 M	3.0
3	0.5 L of 0.2 M disodium hydrogen phosphate	0.1 M	6.5
4	trisodium phosphate	0.1 M	7.0

**Phosphate alpha plots:**

**You-Try-It 6.D****Carbonic Acid**

Table 6.D.1 lists the measured or projected pH of seawater for different levels of atmospheric CO<sub>2</sub>.

- For each solution calculate the fraction of total carbonate that exists as CO<sub>3</sub><sup>2-</sup>. Use this fraction to calculate the equilibrium concentration, [CO<sub>3</sub><sup>2-</sup>]. Do the calculations using K<sub>a</sub> and K<sub>a</sub>' values.

	formula	thermodynamic K <sub>a</sub>	pK <sub>a</sub>	measured (seawater) K <sub>a</sub> '	pK <sub>a</sub> '
carbonic acid	H <sub>2</sub> CO <sub>3</sub>	4.45E-07	6.352	1.45E-06	5.84
hydrogen carbonate ion	HCO <sub>3</sub> <sup>-</sup>	4.69E-11	10.329	1.10E-09	8.96

**Table 6.C.1**

case	seawater	total C <sub>carbonate</sub> (M)	observed p[H <sub>3</sub> O <sup>+</sup> ]	[H <sub>3</sub> O <sup>+</sup> ]
1	average at surface pre-1800	2.3E-03	8.2	6.3E-09
2	average at surface 2000	2.3E-03	8.1	7.9E-09
3	projected average at surface 2100	2.3E-03	7.8	1.6E-08

Carbonate alpha plots using thermodynamic K<sub>a</sub> values:

