Chapter 16: Buffer Calculations

Example 1 - Buffer Method 1

What is the pH of a buffer made by adding 4.68g of sodium benzoate ($NaC_7H_5O_2$) to 250.0mL of 0.15M benzoic acid solution? $K_a = 6.5 \times 10^{-5}$

Need concentration of the conjugate base benzoate ion ($C_7H_5O_2^-$):

$$\left(4.68\text{g } NaC_7H_5O_2\right)\left(\frac{1\text{mol } NaC_7H_5O_2}{144.1\text{g } NaC_7H_5O_2}\right)\left(\frac{1\text{mol } C_7H_5O_2^-}{1\text{mol } NaC_7H_5O_2}\right) = 0.325\text{mol } C_7H_5O_2^-$$

$$\left[C_7H_5O_2^-\right] = \frac{0.0325\text{mol } C_7H_5O_2^-}{0.25\text{L}} = 0.13\text{M } C_7H_5O_2^-$$

	$HC_7H_5O_2$	+	H_2O	⇔	H_3O^+	+	$C_7H_5O_2^-$
I					0		
C					+x		
E					x		

$$K_a = \frac{[H_3O^+][C_7H_5O_2^-]}{[HC_7H_5O_2]}$$

CHECK: Henderson - Hasselbalch Equation

If assume x is small compared to initial concentrations of acid and conjugate base, one can use the initial values of the acid and conjugate base for equilibrium concentrations.

$$K_a = \frac{[H^+][A^-]}{[HA]}$$

$$[H^+] = \frac{K_a[HA]}{[A^-]}$$

$$-\log[H^+] = -\log K_a - \log\left(\frac{[HA]}{[A^-]}\right)$$

$$pH = pK_a + \log\left(\frac{[A^-]}{[HA]}\right)$$

$$pH = pK_a + \log\left(\frac{[\text{base}]}{[\text{acid}]}\right)$$

pH =

Example 2 - Buffer Method 2

What is the pH of a buffer made by adding 125mL of 0.14M $HC_7H_5O_2$ solution with 165mL of 0.16M $NaC_7H_5O_2$ solution? $K_a = 6.5 \times 10^{-5}$

Need concentrations of the conjugate acid and base in the mixture.

	$HC_7H_5O_2$	+	H_2O	$\Leftrightarrow$	H_3O^+	+	$C_7H_5O_2^-$
I					0		
C					+x		
E					x		

$$K_a = \frac{[H_3O^+][C_7H_5O_2^-]}{[HC_7H_5O_2]}$$

CHECK: $\text{pH} = pK_a + \log\left(\frac{[\text{base}]}{[\text{acid}]}\right) =$

Example 3 – Buffer Range

At what pH does buffer work best? Best buffer system when $pH = pK_a$

What is the range of a buffer? Buffer works within ±1 of pK_a value so buffer $pH = pK_a \pm 1$

What is the buffer range of benzoic acid/benzoate buffer?

$pK_a = -\log(6.5\times10^{-5}) = 4.19$ Buffer range = 4.19 ± 1 so 3.19 to 5.19

What is the pH for best buffer capacity and what is the buffering range for each of the following?

Buffer components	pH best buffering capacity	Buffer range
$HC_2H_3O_2$ / $C_2H_3O_2^-$		
$HClO$ / ClO^-		
HCO_3^- / CO_3^{2-}		
$HCHO_2$ / CHO_2^-		
NH_4^+ / NH_3		

Example 4 –Addition of base to buffer
What is the new pH if 5.0 mL of 0.50M NaOH is added to 50.0mL of benzoic acid-benzoate buffer from problem 1?

$[HC_7H_5O_2] = 0.15M$ $[C_7H_5O_2^-] = 0.13M$

First determine how much buffer reacts since NaOH is a strong base, NaOH will react 100% with the acid component of the buffer. MUST WORK STOICHIOMETRY IN MOLES.

	$HC_7H_5O_2$	+	$NaOH$	–>	H_2O	+	$NaC_7H_5O_2$
	(0.0500L x 0.15M)		(0.0050L x 0.50M)				(0.0500L x 0.13M)
Initial mol							
Reaction							
Final mol							

Note: Must divide by the total volume before entering new values into ICE chart.
Total volume = 50.0 mL + 5.0 mL = 55.0 mL or 0.0550L

$[HC_7H_5O_2]=$ $[C_7H_5O_2^-]=$

	$HC_7H_5O_2$	+	H_2O	⇔	H_3O^+	+	$C_7H_5O_2^-$
I					0		
C					+x		
E					x		

$$K_a = \frac{[H_3O^+][C_7H_5O_2^-]}{[HC_7H_5O_2]}$$

CHECK: $$pH = pK_a + \log\left(\frac{[base]}{[acid]}\right) =$$

Example 5 –Addition of acid to buffer
What is the new pH if 10.0 mL of 0.15M HCl was added to 50.0mL of benzoic acid-benzoate buffer from problem 1?

$[HC_7H_5O_2] = 0.15M$ $[C_7H_5O_2^-] = 0.13M$

First determine how much buffer reacts since HCl is a strong acid, HCl will react 100% with the base component of the buffer. MUST WORK STOICHIOMETRY IN MOLES.

	$NaC_7H_5O_2$	+	HCl	–>	$HC_7H_5O_2$	+	$NaCl$
	(0.0500L x 0.13M)		(0.010L x 0.15M)		(0.0500L x 0.15M)		
Initial mol							
Reaction							
Final mol							

Note: <u>Must divide by the total volume before entering new values into ICE chart</u>.
Total volume =

	$HC_7H_5O_2$	+	H_2O	$\Leftrightarrow$	H_3O^+	+	$C_7H_5O_2^-$
I					0		
C					+x		
E					x		

$$K_a = \frac{[H_3O^+][C_7H_5O_2^-]}{[HC_7H_5O_2]}$$

CHECK: $\quad pH = pK_a + \log\left(\frac{[\text{base}]}{[\text{acid}]}\right) =$

Example 6 – Depleting buffer
How much of the 0.15M HCl would have to be added to 50.0 mL of the benzoic acid/benzoate buffer to deplete it completely?

$[HC_7H_5O_2] = 0.15M \qquad [C_7H_5O_2^-] = 0.13M$

Since an acid added to a buffer will act with the conjugate base, determine how much acid will be required to react with 50.0 mL of 0.13M $C_7H_5O_2^-$.

	$NaC_7H_5O_2$	+	HCl	–>	$HC_7H_5O_2$	+ NaCl
	(0.0500L x 0.13M)		(? L x 0.15M)		(0.0500L x 0.15M)	
Initial mol	0.0065 mol		0.0065 mol		0.0075 mol	
Reaction	– 0.0065 mol		– 0.0065 mol		_______ mol	
Final mol	0 mol		0 mol		mol	

Buffer would be depleted when _______ mL of 0.15M HCl has been added.
At this point only acid $HC_7H_5O_2$ remains. <u>Note: can NOT use Henderson-Hasselbalch equation since NO longer a buffer.</u>

$[HC_7H_5O_2] = \frac{\quad\text{mol}}{\text{L}} =$ $\qquad$ Volume = 50. mL + _____ mL =

	$HC_7H_5O_2$	+	H_2O	⇔	H_3O^+	+	$C_7H_5O_2^-$
I					0		
C					+x		
E					x		

$$K_a = \frac{[H_3O^+][C_7H_5O_2^-]}{[HC_7H_5O_2]}$$

Likewise, similar calculation can be done for depletion of acid component of buffer.

Example 7 – Determining acid/base ratio needed for buffer pH

When need to know either
(A) how much of one of the buffer components to add to produce a certain pH or
(B) what ratio of conjugate base to acid is needed to produce a certain pH,
<u>use Henderson-Hasselbalch equation</u>.

How many grams of sodium benzoate ($NaC_7H_5O_2$) must be added to 100. mL of 0.13M benzoic acid ($HC_7H_5O_2$) to produce a buffer with a pH of 4.30?

$K_a = 6.5 \times 10^{-5}$ $pK_a = -\log K_a = -\log(6.5 \times 10^{-5}) = 4.19$

$$pH = pK_a + \log\left(\frac{[base]}{[acid]}\right)$$

Calculate concentration of base needed to produce pH of 4.30.

Then what mass of base $NaC_7H_5O_2$ is needed to produce desired concentration in 100. mL volume?

To prepare 100. mL of buffer at pH 4.30, measure out ______ g $NaC_7H_5O_2$ and add 0.13M acid $HC_7H_5O_2$ to total volume of 100. mL.

Blood Buffer System

H_2CO_3 conjugate acid (formed when blood gas $CO_2 + H_2O \Leftrightarrow H_2CO_3$)
$Na^+ HCO_3^-$ conjugate base

If add base:
$H_2CO_3 + NaOH \rightarrow H_2O + Na^+ HCO_3^-$
If add acid:
$Na^+ HCO_3^- + HCl \rightarrow H_2CO_3 + Na^+Cl^-$

Cell Buffer System

$H_2PO_4^-$ conjugate acid
HPO_4^{2-} conjugate base

If add base:
$H_2PO_4^- + NaOH \rightarrow H_2O + Na^+ HPO_4^{2}$
If add acid:
$HPO_4^{2-} + HCl \rightarrow H_2PO_4^- + Cl^-$