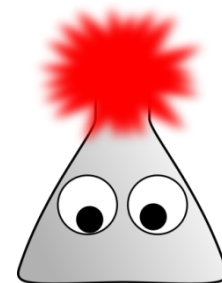


# Buffer Calculations

*It's just equilibrium, it's not magic*

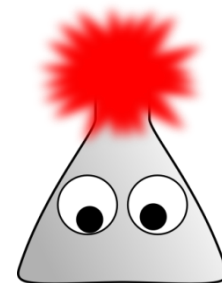


# Calculating Buffers

Buffers are amazingly useful in a wide variety of settings, but they can be a little intimidating.

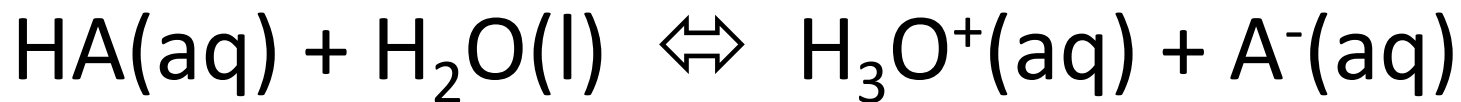
Remember, buffers are just weak conjugate pairs at equilibrium.

For many buffer problems, it is convenient to use the Henderson-Hasselbalch Equation, but where did it come from????



# Acid Dissociation Equilibrium

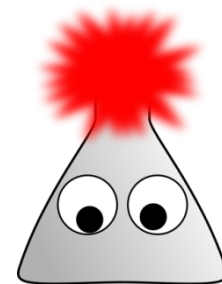
For a generic acid in water we have:



With

$$K_a = \frac{[\text{H}_3\text{O}^+]_{eq}^1 [\text{A}^-]_{eq}^1}{[\text{HA}]_{eq}^1}$$

For buffers, we're usually interested in pH, so let's try to find it in our  $K_a$  expression...



# Finding pH

pH is “ $-\log[H_3O^+]$ ”, so let’s get a “ $-\log$ ” term in there:

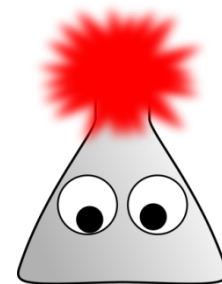
$$-\log K_a = -\log \left( \frac{[H_3O^+]_{eq}^1 [A^-]_{eq}^1}{[HA]_{eq}^1} \right)$$

Recall, “ $-\log X$ ” is “ $pX$ ”

Also recall,  $\log(A * B) = \log A + \log B$ .

So:

$$pK_a = -\log [H_3O^+]_{eq}^1 + \left( -\log \left( \frac{[A^-]_{eq}^1}{[HA]_{eq}^1} \right) \right)$$



# A little rearranging...

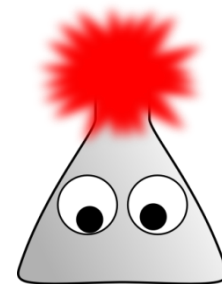
We're getting close...

$$pK_a = -\log[H_3O^+]_{eq}^1 + \left( -\log \left( \frac{[A^-]_{eq}^1}{[HA]_{eq}^1} \right) \right)$$

$$pK_a = pH + \left( -\log \left( \frac{[A^-]_{eq}^1}{[HA]_{eq}^1} \right) \right)$$

$$pK_a + \log \left( \frac{[A^-]_{eq}^1}{[HA]_{eq}^1} \right) = pH$$

$$pH = pK_a + \log \left( \frac{[A^-]_{eq}^1}{[HA]_{eq}^1} \right)$$

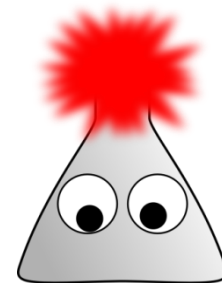


# Henderson-Hasselbalch Equation!

$$pH = pK_a + \log \left( \frac{[A^-]_{eq}^1}{[HA]_{eq}^1} \right)$$

So the H-H Equation is really just  $K_a$ . This also gives us some clues about “good” buffers. If we have an “equimolar” mixture of HA and  $A^-$ , the ratio of their concentrations is 1.  $\log(1)$  is zero, so buffers are “good” when the pH is near the  $pK_a$  of the weak acid.

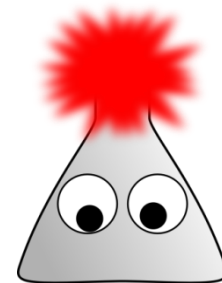
*BONUS: This also gives us a way to find the  $pK_a$  from the titration curve data...*



# Henderson-Hasselbalch Equation!

$$pH = pK_a + \log \left( \frac{[A^-]_{eq}^1}{[HA]_{eq}^1} \right)$$

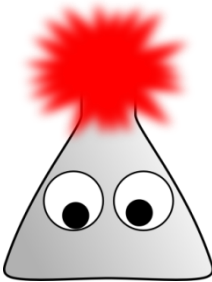
How near the  $pK_a$ ? We said the concentrations should be “within a factor of 10”, so the ratio of concentrations should be less than 10 and more than 0.1.  $\log 10 = 1$ ,  $\log 0.1 = -1$ , so the pH should be within 1 unit of the  $pK_a$  to make an effective buffer.



# Henderson-Hasselbalch Equation!

$$pH = pK_a + \log \left( \frac{[A^-]_{eq}^1}{[HA]_{eq}^1} \right)$$

One warning here... since the concentrations are used in a ratio, we have to be a little careful about them.  $0.01/0.01 = 1$ , and  $100/100 = 1$ , but those would be some VERY different buffers. The concentrations determine the buffer capacity of a buffer. How much acid or base can I add and still be within a factor of 10?





# Henderson-Hasselbalch Equation!

$$pH = pK_a + \log \left( \frac{[A^-]_{eq}^1}{[HA]_{eq}^1} \right)$$

As with everything, using the H-H equation takes some practice. It's a really useful derivation of  $K_a$  when we're working with buffers, but you have to work with it a bit.

Good luck!

