8.6: pH Calculations

One thing that you should notice about the numbers in the previous examples is that they are *very small*. In general, chemists find that working with large negative exponents like these (very small numbers) is cumbersome. To simplify the process, calculations involving hydronium ion concentrations are generally done using *logarithms*. Recall that a **logarithm** is simply the exponent that some base number needs to be raised to in order to generate a given number. In these calculations, we will use a base of 10. A number such as 10,000 can be written as 10^4, so by the definition, the logarithm of 10^4 is simply 4. For a small number such as 10^{-7}, the logarithm is again simply the exponent, or -7. Before calculators became readily available, taking the logarithm of a number that was *not* an integral power of 10 meant a trip to "log tables" (or even worse, using a slide rule). Now, pushing the LOG button on an a scientific calculator makes the process trivial. For example, the logarithm of 14,283 (with the push of a button) is 4.15482. If you are paying attention, you should have noticed that the logarithm contains *six* digits, while the original number (14,283) only contains *five* significant figures. This is because a logarithm consists of two sets of numbers; the digits to the left of the decimal point (called the **characteristic**) simply reflect the integral power of 10, and are *not included* when you count significant figures. The numbers *after* the decimal (the **mantissa**) should have the same significance as your experimental number, thus a logarithm of 4.15482 actually represents *five* significant figures.

There is one other convention that chemists apply when they are dealing with logarithms of hydronium ion concentrations, that is, the logarithm is multiplied by (-1) to change its sign. Why would we do this? In most aqueous solutions, $[H_3O^+]$ will vary between 10^{-1} and 10^{-13} M, giving logarithms of –1 to –13. To make these numbers easier to work with, we take the *negative* of the logarithm (-log$[H_3O^+]$) and call it a ***p*H** value. The use of the lower-case "*p*" reminds us that we have taken the *negative* of the logarithm, and the upper-case "H" tells us that we are referring to the *hydronium ion concentration*. Converting a hydronium ion concentration to a pH value is simple. Suppose you have a solution where $[H_3O^+] = 3.46 \times 10^{-4}$ M and you want to know the corresponding *p*H value. You would enter 3.46×10^{-4} into your calculator and press the LOG button. The display should read "-3.460923901". First, we multiply this by (-1) and get 3.460923901. Next, we examine the number of significant figures. Our experimental number, 3.46×10^{-4} has three significant figures, so our mantissa must have three digits. We round our answer and express our result as, *p*H = 3.461.

The reverse process is equally simple. If you are given a *p*H value of 7.04 and are asked to calculate a hydronium ion concentration, you would first multiply the *p*H value by (-1) to give –7.04. Enter this in your calculator and then press the key (or key combination) to calculate "10^x"; your display should read "9.120108×10^{-8}". There are only two digits in our original mantissa (7.**04**) so we must round this to *two* significant figures, or $[H_3O^+] = 9.1 \times 10^{-8}$.

? Exercise 8.6.1

Calculating $[H_3O^+]$ and pH Values

1. A solution is known to have a hydronium ion concentration of 4.5×10^{-5} M; what is the *p*H this solution?
2. A solution is known to have a *p*H of 9.553; what is the concentration of hydronium ion in this solution?
3. A solution is known to have a hydronium ion concentration of 9.5×10^{-8} M; what is the *p*H this solution?
4. A solution is known to have a pH of 4.57; what is the hydronium ion concentration of this solution?

There is another useful calculation that we can do by combining what we know about *p*H and expression

$$K_W = [H_3O^+][HO^-]$$

We know that $K_W = 10^{-14}$ and we know that (-log $[H_3O^+]$) is *p*H. If we define (-log $[HO^-]$) as *p*OH, we can take our expression for K_W and take the (-log) of both sides (remember, algebraically you can perform the same operation on both sides of an equation) we get:

$$K_W = 10^{-14} = [H_3O^+][HO^-]$$

$$-\log(10^{-14}) = (-\log[H_3O^+]) + (-\log[HO^-])$$

$$14 = pH + pOH$$

Which tells us that the values of *p*H and *p*OH must always add up to give 14! Thus, if the *p*H is 3.5, the *p*OH must be 14 – 3.5 = 11.5. This relationship is quite useful as it allows you to quickly convert between *p*H and *p*OH, and therefore between $[H_3O^+]$ and $[HO^-]$.

We can now re-address *neutrality* in terms of the *p*H scale:

- A solution is **acidic** if *p*H < 7.
- A solution is **basic** if *p*H > 7.
- A solution is **neutral** if *p*H = 7.

The simplest way to determine the *p*H of a solution is to use an electronic *p*H meter. A *p*H meter is actually a sensitive millivolt meter that measures the potential across a thin, sensitive glass electrode that is immersed in the solution. The voltage that develops is a direct function of the *p*H of the solution and the circuitry is calibrated so that the voltage is directly converted into the equivalent of a *p*H value. You will most likely use a simple *p*H meter in the laboratory. The thing to remember is that the sensing electrode has a very thin, fragile, glass membrane and is somewhat expensive to replace. Be careful!

A simple way to estimate the *p*H of a solution is by using an *indicator.* A ***p*H indicator** is a compound that undergoes a change in color at a certain *p*H value. For example, phenolphthalein is a commonly used indicator that is *colorless* at *p*H values below 9, but is *pink* at *p*H 10 and above (at very high *p*H it becomes colorless again). In the laboratory, a small amount of phenolphthalein is added to a solution at low *p*H and then a base is slowly added to achieve neutrality. When the phenolphthalein changes from colorless to pink, you know that enough base has been added to neutralize all of the acid that is present. In reality, the transition occurs at *p*H 9.2, not *p*H 7, so the resulting solution is actually slightly alkaline, but the additional hydroxide ion concentration at pH 9 (10^{-5} M) is generally insignificant relative to the concentrations of the solutions being tested.

A convenient way to estimate the *p*H of a solution is to use *p*H paper. This is simply a strip of paper that has a mixture of indicators embedded in it. The indicators are chosen so that the paper takes on a slightly different color over a range of *p*H values. The simplest *p*H paper is *litmus paper* that changes from pink to blue as a solution goes from acid to base. Other *p*H papers are more exotic. In the laboratory, you will use both indicators, like phenolphthalein, and *p*H papers in neutralization experiments called *titrations* as described in section 8.7.