ORGANIC CHEMISTRY CHEM 12A/B

Logarithm Math and pK_a

Definitions:

log means log_{10} , or "base 10 log" ln (or natural log) means log_e, or "base $e \log$ " where $e \sim 2.718...$

For base 10 log, $\log(10^{\tilde{x}}) = x$ and $10^{\log x} = x$ (e.g., $\log(2365) = 3.374$, so $10^{3.374} = 2365$)

Similarly, for base $e \log$, $\ln(e^x) = x$ and $e^{\ln x} = x$ (e.g., $e^{2.453} = 11.623$, so $\ln(11.623) = 2.453$)

In Chemistry,

 $[H_3O^+] = [H^+] =$ hydronium ion (hydrogen ion) concentration in terms of molarity (M, or mol/L)

 $pH = -log[H_3O^+] = -log[H^+] = negative log base 10 of [H^+]$

If $[H^+] = 1.0 \times 10^{-3} \text{ M}$, then pH = 3.0 (and is a "unitless" number)

If pH = 6.4, then $[H^+] = 1.0 \times 10^{-6.4} M$ (a very small concentration)

 K_{a} , the acidity constant, is defined as:

 $K_{\rm a} = \frac{[{\rm H}^+][{\rm A}^-]}{[{\rm H}{\rm A}]}$ and describes the dissociation for an acid HA shown below:

HA
$$\xrightarrow{K_a}$$
 H⁺ + A⁻

 $pK_a = -\log(K_a)$ and is a useful number to describe the acidity of any acid, especially weak ones.

Acetic acid (CH₃CO₂H) has a p K_a of 4.74 so the value of K_a is $10^{-4.74} = 1.82 \times 10^{-5}$ and is a weak acid.

Negative pK_a means a strong acid (e.g., H_2SO_4 has $pK_a = -3$)

Question 1: How much stronger an acid is trifluoroacetic acid (TFA), pK_a 0.23, compared to acetic acid $(CH_{3}CO_{2}H), pK_{a} 4.74?$

Answer:

The difference in the pK_a 's shows the magnitude. 4.74 - 0.23 = 4.51 "orders of magnitude," so TFA is $10^{4.51}$ (or 32,400) times more acidic than HOAc

Ouestion 2: Derive the Henderson-Hasselbach equation $pH = pK_a + \log [A^-]/[HA]$ from the definition of K_a .