BASICS OF WATER CHEMISTRY

Seachem

general hardness

pH

alkalinity

buffer

carbonate hardness

buffer capacity

dGH

KH

acidity

pH

pH

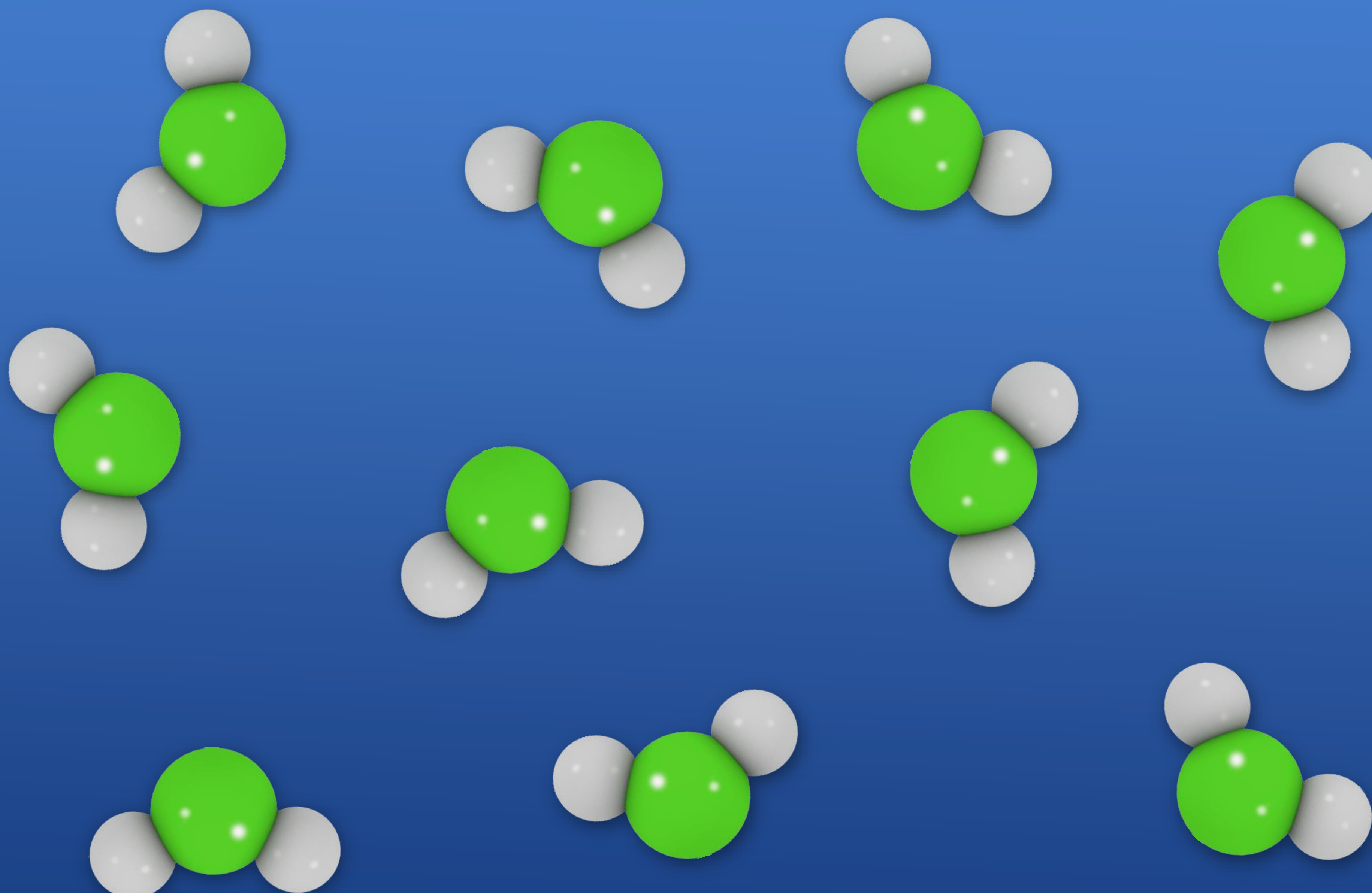
- Representation of relative acidity/basicity of a solution
- Rated on a scale from 0-14
- Low numbers are acidic, high numbers are basic
- pH is dependent on the concentration and activity of hydronium ions (H_3O^+)
  - High hydronium = Low pH
  - Low hydronium = High pH

How pH is Derived

$$pH = -\log_{10} \frac{[H^+]}{1\ mol/L} = -\log_{10} |[H^+]|$$

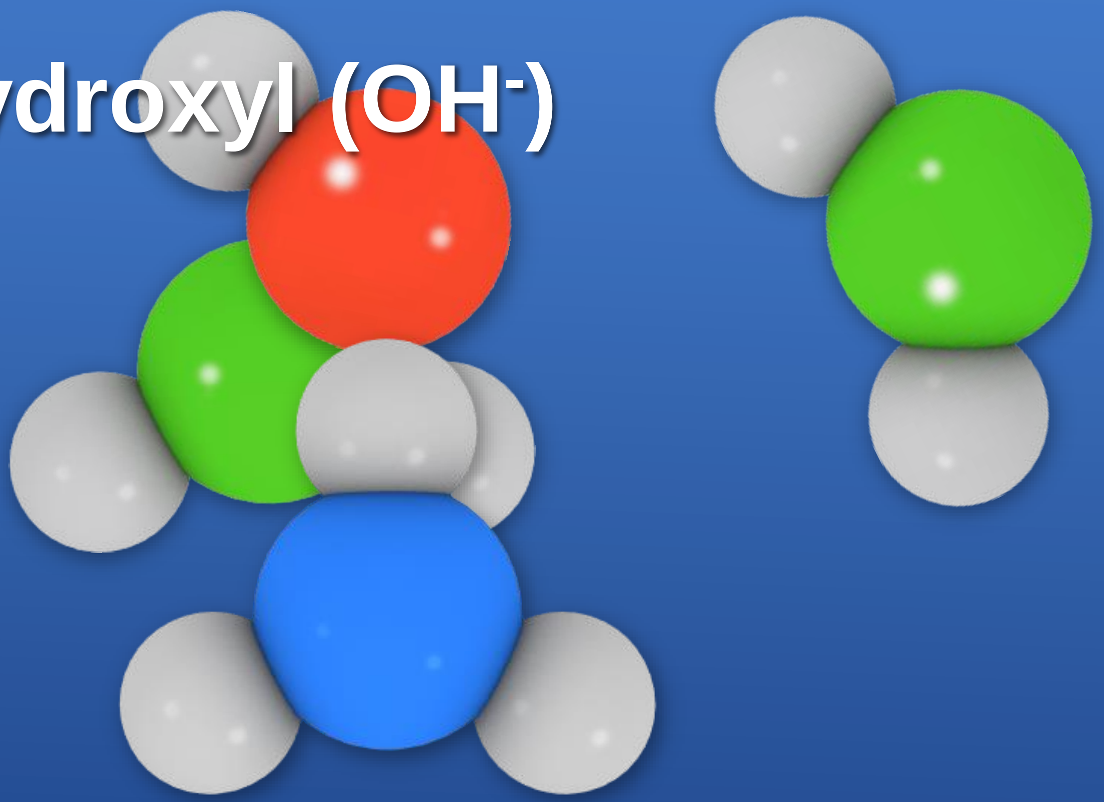
- The pH scale is an inverse logarithmic representation of hydronium concentration
  - each individual pH unit is a factor of 10 different than the next higher or lower unit

H_2O



H_2O dissociation

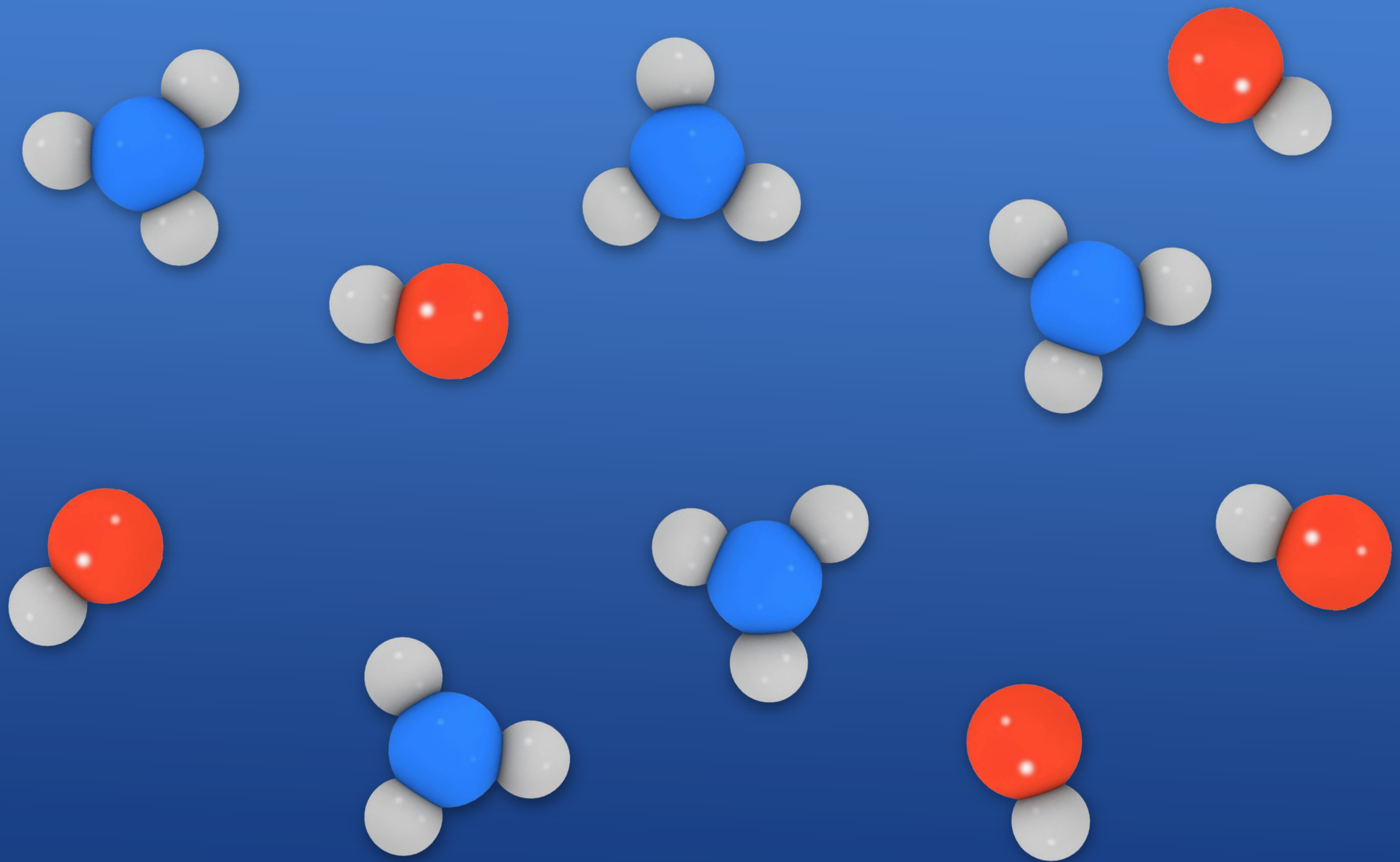
Hydroxyl (OH^-)



Hydronium (H_3O)

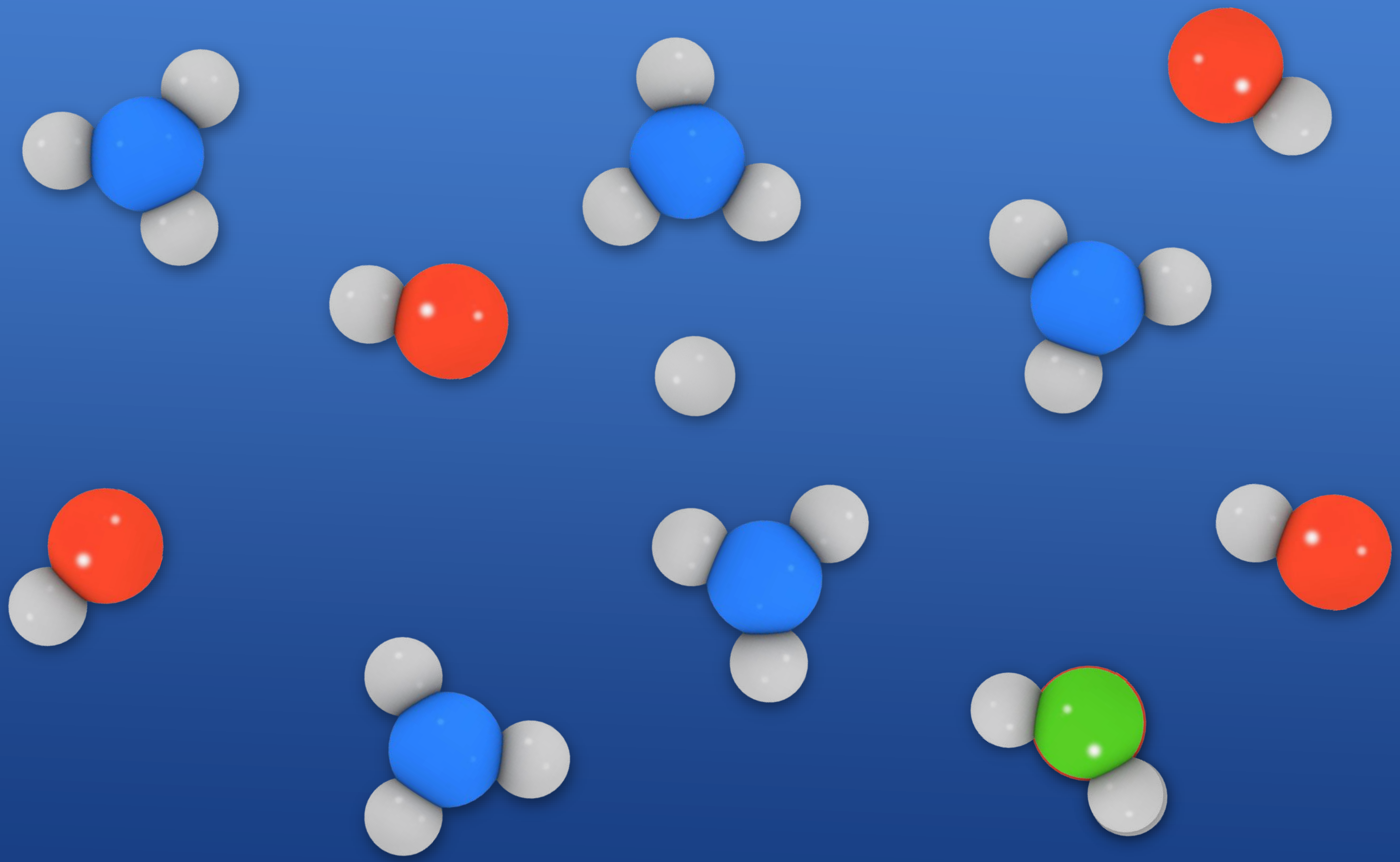
5 hydroniums, 5 hydroxyls

neutral water, pH 7.0



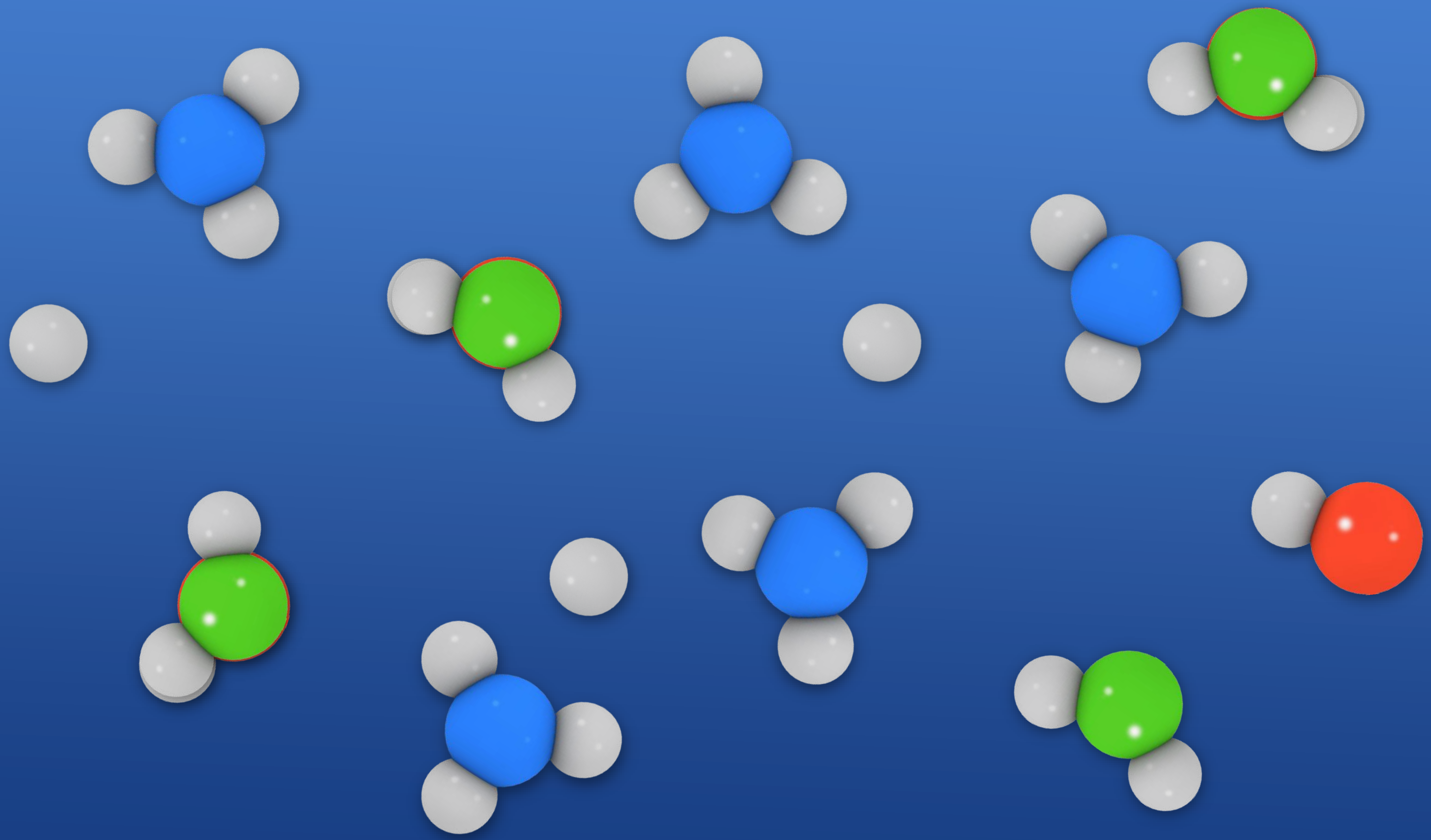
5 hydroniums, 4 hydroxyls

slightly acidic



5 hydroniums, 1 hydroxyl

very acidic



pK_a

pK_a

- K_a is the measure of the strength of an acid
- pK_a (also known as pK) is also the measure of the strength of an acid
- Just as pH is defined as the $-\log[H^+]$, that is, the negative log of the hydrogen ion activity, pK is defined as the $-\log K$
- because it's the -log, lower pK_a values mean a stronger acid

pH and pK_a

- The relationship of pH to pK_a is expressed by the equation:
    - pH = pK + log(base/acid)
- When pH is equal to pK, the buffer is at optimum efficiency
    - This means pH will be least affected by addition of an acid or base

pH and pK_a

if the amount of acid species equals the amount of base species

$$7.0 + \log(6/6) = 7.0$$

now if we add some acid

$$7.0 + \log(6/7) = 6.93$$

but let's say the pK was 6.0, when that acid is added

$$6.0 + \log(6/7) = 5.9$$

the drop in pH is much greater than when the pK was 7.0

BUFFER

Equilibrium

$$A \longrightarrow B$$

$$B \longrightarrow A$$

$$A \underset{k_2}{\overset{k_1}{\longleftrightarrow}} B$$

At equilibrium:

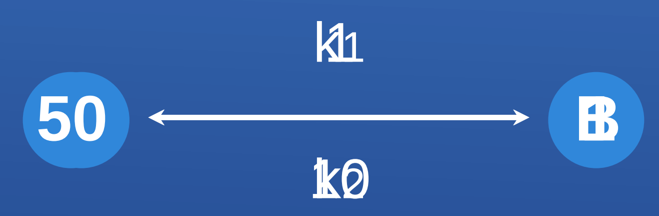
$k_1[A]=k_2[B]$

$k_1/k_2=[B]/[A]$

$\mathbf{K}=[B]/[A]$

Equilibrium

Suppose now that **k1=1** and **k2=10**, and at equilibrium **[A]=10** and **[B]=1**



What happens if we suddenly add enough of A so that
the concentration becomes 50, instead of 10?

LeChâtelier's Principle

$$50 \xleftrightarrow[10]{1} 1$$

$$46.4 \xleftrightarrow[10]{1} 4.6$$

Equilibrium disturbed

Equilibrium restored

when a system at equilibrium is disturbed,
the system will change and adapt to re-establish equilibrium

Buffers

- A buffer is a system of chemical equilibrium that has the effect of stabilizing pH
- An equilibrium mixture of a weak acid and it's conjugate base
- Let's say we have bicarbonate (HCO_3^-) and carbonate (CO_3^{2-}). Bicarbonate is the acid and carbonate is its conjugate base

$$\mathbf{HCO_3^-} \underset{k_2}{\overset{k_1}{\longleftrightarrow}} \mathbf{CO_3^{2-} + H^+}$$

$$k_1[A]=k_2[B]$$

$$k_1[HCO_3^-] = k_2[CO_3^{2-}][H^+]$$

$$\frac{k_1}{k_2} = \frac{[B]}{[A]}$$

$$\frac{k_1}{k_2} = \frac{[CO_3^{2-}][H^+]}{[HCO_3^-]}$$

$$K = \frac{[B]}{[A]}$$

$$K = \frac{[CO_3^{2-}][H^+]}{[HCO_3^-]}$$

acidity can be expressed as $$[H^+] = K * \frac{[HCO_3^-]}{[CO_3^{2-}]}$$

recall that pH is defined as the -log[H+], that is, the negative log of the hydrogen ion activity, and pK is defined as the -logK

ALKALINITY

Alkalinity

- Alkalinity is a measure of the ability of a solution to resist change in pH on the addition of acid
- Alkalinity with acidity constitutes the **buffer capacity**
  - the ability to resist change in pH from either direction
- It is dependent on concentrations of buffering ions in solution
  - Carbonates, Borates, Phosphates, Sulfates, Iodates, Chlorates, etc.

Measuring Alkalinity

- Expressed in one of three units:
  - milliequivalents per liter (meq/L)
  - ~~German degrees of carbonate hardness (dKH)~~
  - ~~parts per million of calcium carbonate (ppm $CaCO_3$)~~
- meq/L is the proper scientific unit of measure
- For purposes of conversion:
  - 1 meq/L = 2.8 dKH = 50 ppm $CaCO_3$

Alkalinity vs. Carbonate Hardness (KH)

- The two are often confused or thought to be the same
  - Carbonate hardness is *only* a measure of carbonates
  - Alkalinity is a measure of *total* acid binding ions
- While not the same, they can be equal
  - If all the alkalinity comes from carbonates and bicarbonates
- Alkalinity is not KH, but KH is alkalinity

HARDNESS

Hardness

- Generally considered to be two types of hardness:
  - General hardness
  - Carbonate hardness
- General hardness is true hardness
- Carbonate hardness technically is not hardness at all, it's alkalinity

General Hardness (GH)

- Measure of dissolved divalent cations, specifically calcium and magnesium
    - Hard water has high levels
    - Soft water has low levels
- Commonly measured in units
    - meq/L
    - German degrees (dH)
    - parts per million of calcium carbonate (ppm $CaCO_3$)

Adjusting Hardness

- General hardness may need to be adjusted:
  - depending on what types of fish or plants you wish to keep
  - if you are using RO or DI water (increase hardness)
  - if your tap water is very hard (decrease hardness)

This concludes Basics of Water Chemistry

Thank You