Introduction

Originally the terms acid and base referred to taste. The practice of classifying substances according to their acidic (sour) or basic (alkaline or bitter) properties dates back to ancient times. An acid was something with a sour taste, such as lemon juice, and a base was something with a bitter taste, such as tonic water. Today there are three additional categories of taste: sweet, salty and umami. The newest, umami, is specific to mono sodium glutamate (MSG).

It is no coincidence that the acid–base properties of compounds are related to taste. Human taste receptors coupled with smell receptors have evolved to interpret certain molecular features as different tastes. Compounds formed from combinations of acids and bases taste salty and are referred to in chemistry as salts. Sweet compounds have characteristics of both acids and bases in the same molecule.

We will explore the relationship between molecular structure and acids–bases, and consider water solutions of acids and bases. In water or a water solution, the solution is acidic if the hydrogen ion concentration is greater than the hydroxide (OH\(^-\)) ion concentration, the solution is basic if the hydroxide ion concentration is greater than the hydrogen (H\(^+\)) ion concentration, and the solution is neutral when the concentrations are equal. Thus the properties of an acid solution are due to the relatively high concentration of hydrogen ion, and the properties of basic solutions are due to the high concentration of hydroxide ions.

As do many of the fundamental ideas in chemistry, the acid–base concept dates back to ancient times and derives from everyday observations about substances people encountered. It was centuries later, however, before molecular interpretations were given to these real-life observations. The acid–base concept is a system of classifying chemical substances which permits both the organization as well as the prediction of a vast number of chemical reactions.

A substance may be assigned to one our four conceivable categories. It may be an acid or a base, but in addition, it may be both an acid and a base or it may be neither an acid nor a base. Early chemists realized that even among acids and bases, some acids were stronger (more sour) or more basic (more bitter) than others. Thus acids may be further classified as strong acids and weak acids, and bases as strong bases and weak bases.

Three Definitions of Acids and Bases
Arrhenius

The Arrhenius definition of acids and bases is the oldest (1884) of the three with which you should be familiar. It derives from Arrhenius’ theories concerning the formation of ions in aqueous solution. It is interesting that he first proposed this idea as a student but his professors considered the idea to be nonsense. As a result he nearly failed to earn the doctorate. He stuck to his convictions, however, and earned a Nobel Prize nineteen years later for this very same insight.

An Arrhenius acid is a hydrogen-containing substance which yields hydrogen ions in aqueous solution. An Arrhenius base is a hydroxyl-containing substance which yields hydroxide ions in aqueous solution. It is obvious from the definitions that for a substance to be an acid in the Arrhenius sense, it must have at least one hydrogen atom, and to be a base, it must have at least one hydroxyl group. Moreover, the Arrhenius definitions only apply to the behavior of substances in water.

Brønsted–Lowry

The Brønsted–Lowry definition of acids and bases liberates the acid–base concept from its limitation to aqueous solutions, as well as the requirement that bases contain the hydroxyl group. A Brønsted–Lowry acid is a hydrogen-containing species which is capable of acting as a proton (hydrogen ion) donor. A Brønsted–Lowry base is a species which is capable of acting as a proton acceptor.

We see that the Brønsted–Lowry acids and bases include those substances that are classified as Arrhenius acids and bases. A substance which yields hydrogen ions is a proton donor, and a substance containing a hydroxyl group which is capable of yielding hydroxide ions in aqueous solution would also be a proton acceptor. Brønsted–Lowry bases, however, are neither required to contain hydroxyl groups nor to form ions in solution.

Lewis

The Lewis definition is the most general of the three. It liberates the acid–base concept from its reliance on the presence of any particular element. It focuses on the behavior of the electrons during an acid–base reaction. The importance of the Lewis definition is that it gets at the basis of acid–base behavior and catalogues the largest number of molecules and reactions. A Lewis acid is an electron pair acceptor; a Lewis base is an electron pair donor.

Conjugate Acids and Bases

The concept of conjugate acids and bases is best understood by considering what happens when a substance behaves as a Brønsted–Lowry acid or a Brønsted–Lowry base. By reversing the reaction in which a substance acts as a proton donor, we see that the product is itself a proton acceptor. It is thus a base, or more specifically, it is the conjugate base of the original acid. Similarly, when a substance behaves as a Brønsted–Lowry base, the product is a proton donor. It is thus the conjugate acid of the original base. In summary, a conjugate base is the species that remains after a Brønsted–Lowry acid donates a proton, and a conjugate acid is the species that forms when a Brønsted–Lowry base accepts a proton.
Glossary

A brief glossary of terms relating the properties of atoms/molecules to acids and bases:

Atomic charge is the charge (usually a fraction) that an atom or group of atoms carries when it is in a molecule. All of the atomic charges in a species must add up to the charge on that species. Atomic charges are important because the charge on an atom in a molecule is its optimal charge. In a reaction if this charge is to be increased or decreased, energy must be supplied. Generally, chemical species that are positively charged are acidic; negatively charged are basic.

Electronegativity is the ability of an atom to attract electrons to itself in a bond. Thus atoms of high electronegativity will acquire excess negative charge (electrons) and will thus have negative atomic charges. They will tend to be bases. On the other hand, atoms of lower electronegativity will then have lost negative charge—electrons—and will have positive atomic charges. They will tend to be acids.

A lone pair or free pair of electrons is a pair of electrons which are in the same orbital. They do not participate in bonding in the molecule. However, they may form a bond with another chemical species that is positively charged, and in so doing act as a base.

A functional group is an atom or group of atoms that has a specific arrangement in an organic molecule. The type of functional group relates to certain chemical properties of that molecule. For example, the –COOH group is referred to as a carboxylic acid. This functional group is the source of acidity in organic acids. Another functional group, the amine, has a nitrogen with a free pair of electrons and behaves as a base.

\[ \text{pH} = -\log [H^+] \]  

\[ \text{pH} = -\log [H_3O^+] \]

It is a scale from 0 to 14. Values <7 are acidic; >7 are basic, and a value =7 is neutral. The pH scale was developed by a Belgian brewmaster to control the quality of his product.

The Water Equilibrium (A critical concept in understanding acid-base behavior)

Pure water is mostly made up of water molecules, but it also consists of very tiny quantities of hydrogen and hydroxide ions in equal amounts. These result from the spontaneous, natural autoionization of water:

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or:

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We can write an equilibrium constant expression for this reaction in the usual manner. It is assigned the symbol \( K_w \) to indicate that it is the equilibrium constant for the autoionization of water:

\[
K_w = [H^+] [OH^-] \text{ or } K_w = [H_3O^+][OH^-] \quad (1.2)
\]

The value of \( K_w \) depends on temperature, as does any equilibrium constant. At 25°C, \( K_w = 1.0 \times 10^{-14} \). Since the dissociation of one water molecule yields one hydrogen ion and one hydroxide ion, their concentrations must be equal in pure water. This allows the calculation of each:

\[
[H_3O^+] = [H+] = [OH^-] = 1.0 \times 10^{-7} \text{ M} \quad (1.3)
\]

Water solutions, composed of solutes dissolved in water, do not necessarily have equal hydrogen ion and hydroxide ion concentrations. Such solutions will still follow Equation 18.2, however, and the product of the concentrations of the hydrogen and hydroxide ions will equal \( 1.0 \times 10^{-14} \) at 25°C.

The pH Scale

Working with the tiny numbers associated with hydrogen ion and hydroxide ion concentrations in solutions can be awkward. For convenience, chemists often work with base-10 logarithms, which are referred to as "p" numbers. This allows concentrations to be expressed as numbers that generally range between 1 and 14. If \( Z \) is a value, then, by definition

\[
pZ = -\log Z \quad (1.4)
\]

When applied to hydrogen ion and hydroxide ion concentration, we have

\[
pH = -\log [H+] = -\log [H_3O^+] \text{ and } pOH = -\log [OH^-] \quad (1.5)
\]

Working in the other direction, if \( pH \) or \( pOH \) is known and hydrogen ion or hydroxide concentration is wanted,

\[
[H_3O^+] = [H+] = 10^{-pH} \text{ and } [OH^-] = 10^{-pOH} \quad (1.6)
\]

Weak Acid Equilibria

A weak acid is a hydrogen-bearing molecular compound that ionizes only slightly in water solution. Using \( HX(aq) \) as the formula of a weak acid dissolved in water, the ionization equilibrium is
HX (aq) H⁺ (aq) + X⁻(aq) \text{(1.7)}
H₂O (l) + HX (aq) H₃O⁺ (aq) + X⁻(aq)

and the associated equilibrium expression is

\[ K_a = (1.8) \]

\( K_a \) is the equilibrium constant for the acid. The concentration of the undissociated acid, HX, is much greater than the concentrations of hydrogen ion and the conjugate base of the weak acid, X⁻. Therefore, weak acid equilibrium constants have values less than one. The weaker the acid, the smaller the value of the equilibrium constant. \( K_a \) values for many common weak acids are available in reference books and general chemistry textbooks.

Another important concept arises from the fact that weak acids dissociate only slightly: The amount of weak acid that ionizes is usually negligible when compare with its initial concentration. To illustrate, consider a 0.10 M solution of a weak acid. If this acid is 2.0% dissociated at equilibrium, 0.10 \times 0.020 = 0.0020 moles of acid per liter of solution are ionized. Applying the rules of significant figures, 0.10 M – 0.0020 M = 0.10 M of acid remains undissociated, which is the initial concentration. Thus, you can see that the amount that ionizes is not significant, and the initial acid concentration essentially is unchanged by the dissociation.

The concentrations of hydrogen ion and conjugate base of the weak acid cannot be neglected in weak acid equilibria. In fact, determining these concentrations is frequently the goal of theoretical calculations and experimental investigations of weak acid solutions. If the weak acid solution is not combined with any other compound, [H₃O⁺] = [H⁺] = [X⁻] because each comes from the same source, the dissociation of HX (aq).

Worksheets

- Acids and Bases: Worksheet #1
- Acids and Bases: Worksheet #2
- Acids and Bases: Worksheet #3

Outside Links

- http://www.zoology.ubc.ca/~auld/bio3...ory_taste.html

Reference

- Tutorial: http://www.science.ubc.ca/~chem/tutorials/pH/

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