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Ageneral Approach to The Buffer Function and Buffer Behavior

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Abstract: Buffering systems are widely used in all fields of science that involve the use of aqueous solutions, such as pharmaceuticals, environmental and analytical chemistry. However, there are several approaches and parameters that can be used to try to explain buffering behavior, such as Van Slyke buffer value, Kolthoff's buffer capacity, acidity, alkalinity, etc., but they cannot provide a global explanation. In this article, we propose the buffering function, which is the basic equation that allows us to explain all types of buffering and the available parameters.

Keywords: Buffer system, Bronsted acid-base theory, concept of pH, Universal buffer, McIlvains buffer, Handerson-Hasselbalch equations, Van Slyke buffer value, Kolthoff buffer capacity, buffer capacity.

Introduction

Buffer systems are very useful in many fields, including chemistry, biochemistry and medicinal, pharmaceutical, industrial, forensic, analytical chemistry, environmental and organic chemistry. A general definition of pH is a solution that resists a change in pH caused by the addition of a Bronsted acid or base. This type of solution usually contains a simple Bronsted acid-base system, and pH resistance occurs in the pH range close to a certain pKa value.

Some buffer solutions contain more than one system, such as McIlvains' buffer (citrate and phosphate); Britton-Robinson; or universal buffer (and its resistance to pH change (or "pH resistance") is difficult to quantify. There are five factors that affect the pH behavior of a buffer solution:

1) Bronsted type of acid-base system (or systems) in solution;
2) concentration of the system;
3) the initial pH value of the solution;
4) the amount of Bronsted acid or base added to the solution that the buffer solution must "counteract";

5) the acceptable pH change after exposure to the buffer solution depending on the application (for example, in an enzymatic system, it should be 0.5 pH units or less). Thus, buffer evaluation parameters must account for all of these factors.

The definition of the buffering function includes some important parameters related to the chemistry of solutions at equilibrium, such as the equilibrium fraction (also called the false mole fraction or dissociation, ionization, or association degree) and the effective electric charge (or simply the effective) requires consideration. charge), taken from the balance of payments. Calculation of buffer concentration (simple or mixed) can be done without using Handerson-Hasselbalch equations. In an equilibrium solution, the electric charge balance must be performed according to the principle of electroneutrality. This means that for a solution of a given pH, the equilibrium positive charge concentration must be equal to the equilibrium negative charge concentration. The concentration of electric charge due to ion i, which represents its contribution, is equal to the product of its charge (qi) and the equilibrium concentration. Thus, the electric charge balance is expressed by the sum of all contribution terms

$$\sum qi[i]=0$$

The equilibrium concentration of a chemical species in the Bronsted acid-base system is directly related to its analytical concentration (c) (or the analytical concentration of the system), taking into account its equilibrium fraction (α). This parameter, in turn, depends only on the pH value of the solution and the pKa values for the Bronsted acid-base system.

$$a_{f(i)}=\frac{[i]}{c(i)}$$

An important application of the buffering function is the estimation and prediction of the buffering effect in solutions with multiple Brønsted acid-base systems, such as mixed buffer solutions. This function allows easy calculations for this type of solution, for example, when choosing suitable systems for mixing under certain experimental conditions. Since the function t takes into account the sum of the contributions of all systems in solution, the calculation of buffer strength can be performed over a wide pH range, as well as a graphical evaluation.

Buffer Capacity (qDc) Buffer capacity describes the amount of acid or base required to change the pH between two values (initial and final values). Since the charge balance is determined for each pH state, this parameter can be calculated by taking into account the difference between the charge balances at each pH. Therefore, it can be expressed (and defined) as the difference in the buffering function, where the subscripts A and B indicate the final (after pH change) and initial (buffer solution) pH values, respectively. Buffer strength is a particularly important and practical parameter because it represents the effective effect of changing the analyte concentration or pH of the systems present in solution. In the case described above, the buffer capacity for each solution can be directly calculated. Thus, the Kolthoff buffer capacity is a special case of buffer strength (and buffer function) when the change in pH is equal to unity.

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Buffer solutions of some substances

Substance	pH
0.05M potassium tetra oxalate dihydrate solution ($KH_3C_4H_4O_8*2H_2O$; M.m 259.19	1.679 (25° C)
Saturated solution of potassium hydrotartrate (0.025M) ($KHC_4H_4O_6$; M.m 188.178)	3.567(25°C)
0.05M potassium dihydrocitrate ($KH_2C_6H_5O_7$; M.m 230.215)	3.776(25°C)
0.05 Potassium hydrophthalate solution ($KHC_8H_4O_4$; M.m204.223)	4.008(25°C)
Saturated solution of piperazine phosphate(=0.065M) $C_4H_{12}N_2HPO_4*H_2O$); M.m202.147)	6.36(16°C); 6.34(18°C)
0.05M sodium tetraborate solution ($Na_2B_4O_7*10H_2O$; M.m381.372)	9.18(25°C); 9.07(38°C)

The most commonly used buffer mixtures are the following

The name of the mixture	Content	pH
With formate	A mixture of formic acid HCOOH and sodium formate HCOONa.	3.8
Benzoate	A mixture of sodium benzoate C_6H_5OONa with benzoic acid C_6H_5OOH.	4.2
Acetate	A mixture of CH_3COONa with acetic acid CH_3COOH.	4.8
Ammonium	Mixture of ammonium chloride NH_4Cl with ammonia NH_4OH.	9.2
Phosphate	Sodium dihydrogen phosphate NaH_2PO_4 with sodium hydrogen phosphate $NaHPO_4$	6.6

Based on the above information, in practice, it is possible to optimally change the concentrations of weak acid and its salt, weak base and its salt in buffer solutions, and create buffer solutions with the required pH value.

The hydrogen index of buffer solutions can be measured in several different ways: colorimetric, conductometric and potentiometric.

In the potentiometric method, pH is determined using a galvanic element in which one of the electrodes (serving as an indicator) is resistant to hydrogen ions, and the other has a constant potential that does not depend on the properties of the studied solution.

A buffer solution (more precisely, pH buffer or hydrogen ion buffer) is an aqueous solution consisting of a mixture of a weak acid and its conjugate base, or vice versa. When a small amount of a strong acid or base is added to it, its pH changes very little. Buffer solutions are used in various chemical applications as a means of maintaining the pH value at a nearly constant value. There are many living systems in nature that use buffering to regulate pH. For example, the bicarbonate buffering system is used to regulate blood pH, and bicarbonate also acts as a buffer in the ocean.

There are several parameters that can be used to describe different aspects of buffering solutions or buffering effects. All these parameters can be obtained using the buffering function (t), which provides a more complete evaluation of the system. Using this function, the Van Slyke buffer value, Kolthoff buffer capacity, and buffer capacity parameters can be compared and confusion about the Kolthoff parameter can be identified. The buffering function can more fully explain the effects of pH related to various conditions or parameters, such as acid-base titration, alkalinity, acidity, base (or acid) neutralizing capacity, or even the pH of pure solutions. Finally, it can be easily detected using a common computer software package.

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