# From p*K*a to the pH of weak base solutions

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## ABSTRACT

Undergraduate biochemistry students frequently find the quantitative treatment of weak acids and bases troublesome. Given the p*K*a of a weak acid *HA*, for instance, many students struggle to calculate the pH of a solution of the conjugate base *A*– at concentration *C*, . The traditional method involves calculating the base dissociation constant *K*b and the artificial quantity pOH before reaching pH, but these steps increase the risk of mistakes and provide little insight into acid-base equilibria. The alternative method presented here allows students to calculate the pH of a weak base solution from the p*K*a of its conjugate acid without calculating *K*b and pOH, using a memorable relationship:

## RUNNING TITLE

pH of weak bases

## KEYWORDS

Biological chemistry, acids and bases, aqueous solutions, calculations.

## INTRODUCTION

The biochemical importance of weak acids and bases makes them prominent in introductory chemistry courses, but students often find their quantitative treatment difficult [1]. Conjugate acid-base analysis begins with the observation that the ionic product of water, *K*w, is exactly equal to 1.0×10-14 at 25 °C [2]. The central role of water in the acid-base chemistry of dissolved substances leads to the well-known eqns. 1 and 2 [2]:

 (1)

 (2)

where *K*a is the acid dissociation constant of a weak acid (HA), *K*b is the base dissociation constant of the same same acid’s conjugate base (A–), and the function p(x) = –log10(x).

## CALCULATING THE pH OF A WEAK ACID

Weak acids present few conceptual problems to biochemistry students. A weak Brønsted-Lowry acid, like a strong Brønsted-Lowry acid, lowers the pH of a solution by transferring its own protons into solution. First-year undergraduate students are usually taught to calculate the pH of a dilute solution of a weak monoprotic acid by an approximate procedure which relies on three assumptions: 1) the acidity of the solution is dominated by the dissolved acid, 2) the acidity of water is inconsequential, and 3) HA dissociates to a negligible extent [3]. If these assumptions hold, a student can follow introductory textbooks in using eqns. 3 and 4 to calculate the pH:

 (3)

 (4)

 where pH(HA, *C*) is the pH of a solution of HA at molar concentration *C*. As long as these equations’ limitations are understood then they serve students well, and along with the Henderson-Hasselbalch equation [4] are easily applied to biochemical and pharmacological problems.

## WEAK BASE CALCULATIONS

Students find it harder to calculate the pH of a weak base solution than a weak acid solution. They must first must overcome a conceptual barrier which stops them from easily connecting the problem with their knowledge of strong Arrhenius bases. While a strong base raises the pH of a solution in a way that is analogous to the action of an acid – by transferring its own hydroxide ions into solution – a weak Brønsted-Lowry base raises the pH of a solution in an indirect way, by receiving protons from water [5]. This “passive” basicity of weak bases cannot be understood apart from the acidity of water, and students cannot form a straightforward conceptual link with the “active” basicity of strong bases. The difficulty is both demonstrated and caused by inconsistencies in the way weak bases such as ammonia are introduced in textbooks [5].

The second difficulty is one of convention. Because the weak acidity and weak basicity of a conjugate pair are symmetrically connected by their reactions with water, and are really two aspects of the same phenomenon, biochemists and pharmacologists use p*K*a values to describe the basicity of weak bases [6]. While this is desirable from the point of view of simplifying terminology, from the student’s point of view this acidocentric viewpoint can pose problems. When a p*K*a value is provided in the context of a particular exercise, students must carefully decide whether a protonation or a deprotonation reaction is taking place [7]. At its worst, an acidocentric approach to bases leads to confusion: “for a weak base, B, the ionization reaction is BH+ ⇌ B + H+ and the dissociation constant p*K*a is given by the Henderson-Hasselbalch equation” [8].

## CALCULATING THE pH OF A WEAK BASE

If a student successfully recognizes that the problem involves the protonation of a weak base, despite having been given the p*K*a of its conjugate acid, then he/she may calculate the approximate pH of the basic solution as follows:

1. Write down the weak base equilibrium according to eqn. 5:

 (5)

1. Use eqns. 1 and 2 to find *K*b
2. Use eqns. 6 and 7 (which are basic versions of eqns. 3 and 4) to calculate the pOH of the solution, where *C* is the molar concentration of A–:

 (6)

 (7)

1. Use eqn. 8 to find the pH of the solution:

 (8)

where pH(A–, *C*) is the pH of a solution of A–at concentration *C*.

This procedure is complicated enough to be difficult for many students. The question “given this p*K*a, what is the pH?” is formulated in acidic terms, but the student must translate the problem into basic terms to arrive at the artificial quantity pOH before reaching the final answer. The process recapitulates the method used for a weak acid but in a lengthened and awkward form. As a reward for this work the student receives little or no compensatory insight into the behavior of weak bases.

## ANOTHER WAY TO CALCULATE THE pH OF A WEAK BASE

The present author proposes an alternative method which allows students to calculate the pH of a weakly basic solution from the p*K*a of its conjugate acid without calculating *K*b and pOH. The key relationship is given in eqn. 9:

 (9)

where pH(HA, *C*) is the pH of weak acid HA at concentration *C*, and pH(A–, *C*) is the pH of weak base A– at the same concentration *C*. This relationship depends on the same assumptions, and is therefore valid under the same range of conditions, as eqns. 3, 4, 6 and 7.

Using this relationship, a student who is given the p*K*a of a weak acid HA and asked to calculate the pH of a solution of its conjugate base A– at concentration *C* may follow this procedure:

1. Use eqns. 3 and 4 to calculate the pH of a solution of HA at concentration *C*
2. Use eqn. 9 to find the pH of the solution A– at concentration *C*.

This procedure is less complex than the traditional procedure (eqns. 5-8) and, in the present author’s experience, leads students more safely to the same answer. The method does not preclude students from learning the significance of eqn. 5 and the meaning of *K*b, and they may use eqn. 9 alongside traditional procedures to check their answers.

## DERIVATION OF EQN. 9

Expanding eqn. 4 gives eqn. 10:

 (10)

The definition of the p function allows us to write eqn. 11, which in turn gives eqn. 12, an expression for the pH of a weak acid solution in terms of its p*K*a.

 (11)

 (12)

We now derive the equivalent expression for pH(A–, *C*a). Combining eqns. 7 and 8 yields eqn. 13:

 (13)

Using eqn. 1 to substitute *K*a for *K*b gives eqn. 14:

 (14)

Expanding eqn. 14 gives eqn. 15:

 (15)

Eqn. 15 written in terms of the p*K*a (using eqn. 11) gives us our final basic pH expression, eqn. 16:

 (16)

We can now add together the eqns. 12 and 16 to yield eqn. 17, which simplifies to eqn. 9.

 (17)

## CONCLUSION

Weak bases are ubiquitous in biochemistry and pharmacology, but the way undergraduate students are taught to calculate the pH of a weak base from the p*K*a of its conjugate acid is complex and prone to error. I present here another method, eqn. 9, by which students may reach the answer without first having to calculate *Kb* and pOH. As long as students understand the conceptual importance of the weak base equilibrium (eqn. 5) then any secure way of calculating a weak base’s pH is valuable, and eqn. 9 makes a useful addition to a student’s armoury.

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