Key for Acid/Base Properties of a Pharmaceutical Compound

Many pharmaceutically interesting compounds are weak acids or weak bases, a fact of some importance when they are prepared for use by the public. For example, if the active ingredient in a nasal spray is too acidic, then the preparation might include an additional ingredient to neutralize some of the acid; after all, no one wants to spray something as acidic as, say, lemon juice up his or her nose!

Pseudoephedrine is a central nervous system stimulant used in many cold and allergy tablets. In its molecular form it is a weak base (it is an amine), which, for convenience, we may represent as B. In water, the following equilibrium reaction exists

$$B(aq) + H_2O(l) \rightleftharpoons OH^-(aq) + HB^+(aq)$$

The Merck Index reports that a 0.030 M solution of pseudoephedrine has an equilibrium pH of 11.44. What is the value of K_b for this compound?

Answer. With a pH of 11.44, the pOH is 2.56 and the equilibrium concentration of OH^- is 2.75×10^{-3} M. We can enter this value into an ICE table where the values in **bold** serve as our starting point.

	В	+	$\mathrm{H}_{2}\mathrm{O}$	\rightleftharpoons	OH-	+	HB^+
initial	0.030				0		0
change	$-2.75 imes10^{-3}$				$+2.75 imes10^{-3}$		$+2.75 imes10^{-3}$
equilibrium	0.02725		—		$2.75 imes \mathbf{10^{-3}}$		2.75×10^{-3}

Substituting the equilibrium concentrations into the K_b expression gives its value as

$$K_b = \frac{[\text{HB}^+][\text{OH}^-]}{[\text{B}]} = \frac{(2.75 \times 10^{-3})^2}{0.02725} = 2.77 \times 10^{-4}$$

Because its base form is only slightly soluble in water, pseudoephedrine typically is dispensed in its weak acid form as pseudoephedrine hydrochloride. Although the compound ofent is written as $B \cdot HCl$, it actually consists of the ions HB⁺ and Cl⁻. A solution of pseudoephedrine hydrochloride is acidic due to the presence of HB⁺. Write the K_a reaction that is responsible for making the solution acidic and report the value for K_a .

Answer. The reaction is $HB^+(aq) + H_2O(l) \rightleftharpoons H_3O^+(aq) + B(aq)$ for which the equilibrium constant is

$$K_a = \frac{K_w}{K_b} = \frac{1.00 \times 10^{-14}}{2.77 \times 10^{-4}} = 3.61 \times 10^{-11}$$

Suppose you dissolve three tablets of Sudafed[®], each containing 30.0 mg of pseudoephedrine hydrochloride, in 200.0 mL of water. What is the pH of the resulting solution? The molar mass for pseudoephedrine hydrochloride is 201.7 g/mol.

Answer. We begin by finding the concentration of pseudoephedrine hydrochloride, which is

$$\frac{3 \text{ tablets} \times \frac{0.030 \text{ g}}{\text{tablet}} \times \frac{1 \text{ mol}}{201.7 \text{ g}}}{0.200 \text{ L}} = 2.23 \times 10^{-3} \text{ M}$$

Taking this as the initial concentration of HB⁺, we use an ICE table to help us set up the problem

	HB^+	+	$\rm H_2O$	\rightleftharpoons	$\mathrm{H}_{3}\mathrm{O}^{+}$	+	В
initial	2.23×10^{-3}				0		0
change	-x				+x		+x
equilibrium	$2.23 \times 10^{-3} - x$				x		x

$$K_{a} = \frac{[\mathrm{H}_{3}\mathrm{O}^{+}][\mathrm{B}]}{[\mathrm{HB}^{+}]} = \frac{x^{2}}{2.23 \times 10^{-3} - x} = 3.61 \times 10^{-11}$$
$$2.23 \times 10^{-3} - x \approx 2.23 \times 10^{-3}$$
$$K_{a} = \frac{x^{2}}{2.23 \times 10^{-3}} = 3.61 \times 10^{-11}$$
$$x = 2.84 \times 10^{-7}$$

Checking the assumption—left as an exercise for you—gives an error of 0.01%, which is an acceptable error; thus, the $[H_3O^+]$ is 2.84×10^{-7} and the pH is 6.55.