Types of pH Calculations in Aqueous Solution (rev. D 4/2/2025)

It is best to think of acids and bases in Bronsted-Lowry terms.

1. The simplest situation is a strong acid in water. Use the definition of pH and the convention that the hydronium ion activity is equal to the acid concentration, because of 100% dissociation. Use HA as the formula for a strong acid.

   $HA_{(aq)} + H_2O_{(l)} \text{->} H_3O^+_{(aq)} + A^-_{(aq)}$

   $pH = - \log [H_3O^+] = - \log [HA]$

2. This also works for strong bases. Use B as the formula for a strong base.

   $B_{(aq)} + H_2O_{(l)} \text{->} OH_{-(aq)} + BH^+_{(aq)}$

   $pOH = - \log [OH^-] = - \log [B]$

   $pH = 14 – pOH = 14 + \log [B]$

3. For a weak acid in water, the chemical equation is the same, but the acid dissociates less.

   $HA_{(aq)} + H_2O_{(l)} \text{->} H_3O^+_{(aq)} + A^-_{(aq)}$

   $K_a = [H_3O^+] [A^-] / [HA]$

   Create an ICE table

Reaction	[HA]	$[H_3O^+]$	$[A^-]$
Initial	$[HA]_0$	0	0
Change	-x	x	x
Equilibrium	$[HA]_0$ - x	x	x

   $K_a = x^2/([HA]_0 – x)$

   If dissociation is minimal (< 5 %), assume x << [HA]. Be sure to verify after completing calculations.

   $K_a = x^2/[HA]_0$

   $[H_3O^+] = \sqrt{}(K_a[HA]_0)$

$pH = -0.5 \log (K_a[HA]_0)$

If dissociation cannot be ignored:

$K_a = x^2/([HA]_0 – x)$

$(K_a)([HA]_0 – x) = x^2$

$(K_a)[HA_0] – (K_a) x = x^2$

$x^2 + (K_a)x - (K_a)[HA]_0 = 0$

Use *The Quadratic Equation* or a graphing calculator to find the roots! Usually, one of the roots will not make any sense. The correct answer is the other one.

$x = (Ka)/2 +/- sqrt(Ka^2 + 4(K_a)[HA]_0)/2$

$x = [H_3O^+] = [A^-]$

$[HA] = [HA]_0 – x$

4. This also works for weak bases.

$B_{(aq)} + H_2O_{(l)} -> OH-_{(aq)} + BH^+_{(aq)}$

$K_b = [OH^-][BH^+]/[B]_0$

Create an ICE table

Reaction	$[B]$	$[OH^-]$	$[BH^+]$
Initial	$[B]_0$	0	0
Change	-x	x	x
Equilibrium	$[B]_0$ - x	x	x

$K_b = x^2/([B]_0 – x)$

If dissociation is minimal (< 5 %), assume x << [B]. Be sure to verify after completing calculations.

$K_b = x^2/[B]_0$

$[OH^-] = \sqrt{}(K_b[B]_0)$

$pOH = -0.5 \log (K_b[B]_0)$

$pH = 14 – pOH = 14 + 0.5 \log (K_b[B]_0)$

If dissociation cannot be ignored, follow the same calculations as in 3, substituting the appropriate base variables for the original acid ones.

$K_b = x^2/([B]_0 – x)$

$(K_b)([B]_0 – x) = x^2$

$(K_b)[B]_0 – (K_a) x = x^2$

$x^2 + (K_b)x - (K_b)[B]_0 = 0$

Use *The Quadratic Equation* or a graphing calculator to find the roots! Usually, one of the roots will not make any sense. The correct answer is the other one.

$x = [OH^-] = [BH^+]$

$[B] = [B]_0 – x$

5. For a weak acid neutralized by a strong base, at equivalence, assume the conjugate base is dominant, but dissociates slightly.

$A^-{}_{(aq)} + H_2O_{(l)} \text{->} HA_{(aq)} + OH^-{}_{(aq)}$

$K_b = [HA][OH^-]/[A^-]$

Create an ICE table

Reaction	$[A^-]$	[HA]	$[OH^-]$
Initial	$[A^-{}_0$	0	0
Change	-x	x	x
Equilibrium	$[A^-]_0 - x$	x	x

$K_b = x^2/([A^-]_0 - x)$

If dissociation is minimal (< 5 %), assume x << [B]. Be sure to verify after completing calculations.

$K_b = x^2/[A^-]_0$

$[OH^-] = \sqrt{(K_b[A^-]_0)}$

$pOH = -0.5 \log (K_b[A^-]_0)$

$pH = 14 – pOH = 14 + 0.5 \log (K_b[A^-]_0)$

If dissociation cannot be ignored, follow the same calculations as in 3, substituting the appropriate base variables for the original acid ones.

$K_b = x^2/([A^-]_0 – x)$

$(K_b)([A^-]_0 – x) = x^2$

$(K_b)[A^-]_0 – (K_b) x = x^2$

$x^2 + (K_b)x - (K_b)[A^-]_0 = 0$

Use *The Quadratic Equation* or a graphing calculator to find the roots! Usually, one of the roots will not make any sense. The correct answer is the other one.

$x = [OH^-] = [HA]$

$[A^-] = [A^-]_0 – x$

6. For a weak base neutralized by a strong acid, assume the conjugate acid is dominant, but dissociates slightly.

$BH^+_{(aq)} + H_2O_{(l)} \text{->} B_{(aq)} + H_3O^+_{(aq)}$

$K_a = [B][H_3O^+]/[BH^+]_0$

Create an ICE table

Reaction	$[BH^+]$	$[B]$	$[H_3O^+]$
Initial	$[BH^+]_0$	0	0
Change	-x	x	x
Equilibrium	$[BH^+]_0 - x$	x	x

$K_a = x^2/([BH^+]_0 – x)$

If dissociation is minimal (< 5 %), assume $x << [BH^+]_0$. Be sure to verify after completing calculations.

$K_a = x^2/[BH^+]_0$

$[H_3O^+] = \sqrt{(K_a[BH^+]_0)}$

$pH = -0.5 \log (K_a[BH^+]_0)$

If dissociation cannot be ignored, follow the same calculations as in 3, substituting the appropriate base variables for the original acid ones.

$K_a = x^2/(([BH^+]_0 – x)$

$(K_a)([BH^+]_0 – x) = x^2$

$(K_a)[BH^+]_0 – (K_a) x = x^2$

$x^2 + (K_a)x - (K_a)[BH^+]_0 = 0$

Use *The Quadratic Equation* or a graphing calculator to find the roots! Usually, one of the roots will not make any sense. The correct answer is the other one.

$x = [H_3O^+] = [B]$

$[BH^+] = [BH^+]_0 – x$

7. For buffers, use the Henderson-Hasselbalch equation, which is the negative logarithm of the K_a equation, rearranged. Use pK_a for both weak acid and weak base buffers ($pK_a = 14 - pK_b$).

   $pH = pK_a + \log ([A^-]/[HA])$

   $pH = pK_a + \log ([B]/[HB^+])$

   It's all about the ratio.

   If the ratio is > 1, there is more conjugate base than acid, or more base than conjugate acid, and pH is higher than pK_a by the logarithm of the ratio.

   If the ratio is < 1, there is more acid than conjugate base, or more conjugate acid than base, and the pH is less than pK_a by the logarithm of the ratio.

Summary of Formulas, Assuming Dissociation Is Less Than 5 percent						
Type	K_a	pK_a	pH	K_b	pK_b	pOH
Strong acid	$\ge 1x10^{0}$	≤ 1	= - log [HA]	$\le 1x10^{-14}$	≥ 14	= 14 + log [HA]
Salt of weak base			= -0.5 log ($K_a[BH^+]$)			= 14 + 0.5 log ($K_a[BH^+]$)
Weak acid			= -0.5 log (K_a[HA])			= 14 + 0.5 log (K_a[HA])
Buffer			= pK_a + log ($[A^-]$/[HA])			= pKa + log ([B]/$[HB^+]$)
Weak base			= 14 + 0.5 log (K_b[B])			= -0.5 log (K_b[B])
Salt of weak acid			= 14 + 0.5 log ($K_b[A^-]$)			= -0.5 log ($K_b[A^-]$)
Strong base	$\le 1x10_{-14}$	≥ 14	= 14 + log [B]	$\ge 1x10^{0}$	≤ 1	= - log [B]

Rev. B - Corrected errors in Henderson-Hasselbalch formula for base.
Rev. C - Added use of quadratic function to solve 3 and 4.
Rev. D – Expanded 5 and 6 and corrected formulas.

If you find an error, please notify Bill at bvins@mrvins.com!