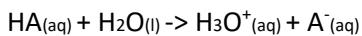


Types of pH Calculations in Aqueous Solution (rev. D 4/2/2025)

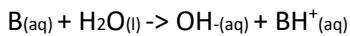
It is best to think of acids and bases in Bronsted-Lowry terms.

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.



$$\text{pH} = -\log [\text{H}_3\text{O}^+] = -\log [\text{HA}]$$

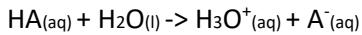
2. This also works for strong bases. Use B as the formula for a strong base.



$$\text{pOH} = -\log [\text{OH}^-] = -\log [\text{B}]$$

$$\text{pH} = 14 - \text{pOH} = 14 + \log [\text{B}]$$

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



$$K_a = [\text{H}_3\text{O}^+] [\text{A}^-] / [\text{HA}]$$

Create an ICE table

Reaction	[HA]	[\text{H}_3\text{O}^+]	[\text{A}^-]
Initial	$[\text{HA}]_0$	0	0
Change	$-x$	x	x
Equilibrium	$[\text{HA}]_0 - x$	x	x

$$K_a = x^2 / ([\text{HA}]_0 - x)$$

If dissociation is minimal (< 5 %), assume $x \ll [\text{HA}]$. Be sure to verify after completing calculations.

$$K_a = x^2 / [\text{HA}]_0$$

$$[\text{H}_3\text{O}^+] = \sqrt{K_a [\text{HA}]_0}$$

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

If dissociation cannot be ignored:

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

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

$$(K_a)[HA_0] - (K_a)x = x^2$$

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

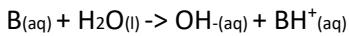
Use *The Quadratic Equation* or a graphing calculator to find the roots! Usually, one of the roots will not make any sense. The correct answer is the other one.

$$x = (K_a)/2 \pm \sqrt{K_a^2 + 4(K_a)[HA]_0}/2$$

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

$$[HA] = [HA]_0 - x$$

4. This also works for weak bases.



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

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.

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

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

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

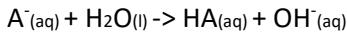
$$x^2 + (K_b)x - (K_b)[B]_0 = 0$$

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.



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

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.

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

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

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

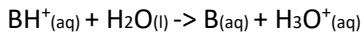
$$x^2 + (K_b)x - (K_b)[A^-]_0 = 0$$

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.



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

Create an ICE table

Reaction	[BH ⁺]	[B]	[H ₃ O ⁺]
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.

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

$$[\text{H}_3\text{O}^+] = \sqrt{K_a [\text{BH}^+]_0}$$

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

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

$$K_a = x^2 / ((\text{BH}^+)_0 - x)$$

$$(K_a)([\text{BH}^+]_0 - x) = x^2$$

$$(K_a)[\text{BH}^+]_0 - (K_a)x = x^2$$

$$x^2 + (K_a)x - (K_a)[\text{BH}^+]_0 = 0$$

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.

$$x = [\text{H}_3\text{O}^+] = [\text{B}]$$

$$[\text{BH}^+] = [\text{BH}^+]_0 - x$$

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 ($pK_a = 14 - pK_b$).

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

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

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	$\geq 1 \times 10^0$	≤ 1	$= -\log [HA]$	$\leq 1 \times 10^{-14}$	≥ 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			$= pK_a + \log ([A^-]/[HA])$			$= pK_a + \log ([B]/[HB^+])$	
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	$\leq 1 \times 10^{-14}$	≥ 14	$= 14 + \log [B]$	$\geq 1 \times 10^0$	≤ 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!