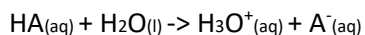


Types of pH Calculations in Aqueous Solution (rev. D 4/2/2025)

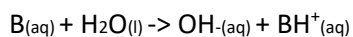
It is best to think of acids and bases in Bronsted-Lowry terms.

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.



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

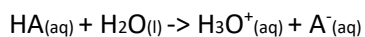
2. This also works for strong bases. Use B as the formula for a strong base.



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

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

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] | [H ₃ O ⁺] | [A ⁻] |
|-------------|-----------------------|----------------------------------|-------------------|
| Initial | [HA] ₀ | 0 | 0 |
| Change | -x | x | x |
| Equilibrium | [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.

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

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

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

If dissociation cannot be ignored:

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

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

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

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

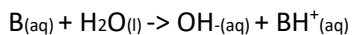
Use *The Quadratic Equation* or a graphing calculator to find the roots! Usually, one of the roots will not make any sense. The correct answer is the other one.

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

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

$$[\text{HA}] = [\text{HA}]_0 - x$$

4. This also works for weak bases.



$$K_b = [\text{OH}^-][\text{BH}^+]/[\text{B}]_0$$

Create an ICE table

| Reaction | [B] | [OH ⁻] | [BH ⁺] |
|-------------|----------------------|--------------------|--------------------|
| Initial | [B] ₀ | 0 | 0 |
| Change | -x | x | x |
| Equilibrium | [B] ₀ - x | x | x |

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

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

$$K_b = x^2 / [\text{B}]_0$$

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

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

$$\text{pH} = 14 - \text{pOH} = 14 + 0.5 \log (K_b[B]_0)$$

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

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

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

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

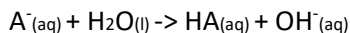
$$x^2 + (K_b)x - (K_b)[B]_0 = 0$$

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.

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

$$[B] = [B]_0 - x$$

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



$$K_b = [\text{HA}][\text{OH}^-] / [\text{A}^-]$$

Create an ICE table

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

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

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

$$K_b = x^2 / [\text{A}^-]_0$$

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

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

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

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

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

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

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

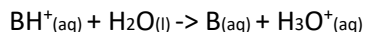
$$x^2 + (K_b)x - (K_b)[A^-]_0 = 0$$

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.

$$x = [\text{OH}^-] = [\text{HA}]$$

$$[A^-] = [A^-]_0 - x$$

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



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

Create an ICE table

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

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

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

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

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

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

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 $\text{p}K_a$ for both weak acid and weak base buffers ($\text{p}K_a = 14 - \text{p}K_b$).

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

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

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 $\text{p}K_a$ 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 $\text{p}K_a$ 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!