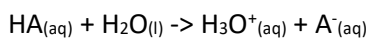


Types of pH Calculations in Aqueous Solution (rev. B 7/25/2024)

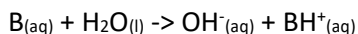
It is best to think of acids and bases in Bronsted-Lowry terms.

1. The simplest situation is for 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.



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

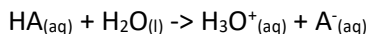
2. This also works for strong bases. Use B as the formula for a strong base.



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

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

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



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

Create an ICE table

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

$$K_a = \frac{x^2}{[\text{HA} - x]}$$

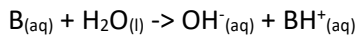
If dissociation is minimal (< 5 %), assume $x \ll [\text{HA}]$. Be sure to verify after completing calculations.

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

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

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

4. This also works for weak bases.



$$K_b = \frac{[OH^-][BH^+]}{[B]}$$

Create an ICE table

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

$$K_b = \frac{x^2}{[B] - x}$$

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

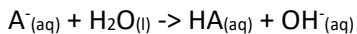
$$K_b = \frac{x^2}{[B]}$$

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

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

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

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



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

Create an ICE table

Reaction	[A ⁻]	[HA]	[OH ⁻]
Initial	[A ⁻]	0	0
Change	-x	x	x
Equilibrium	[A ⁻ - x]	x	x

$$K_b = \frac{x^2}{[A^-] - x}$$

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

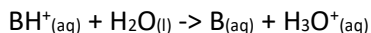
$$K_b = \frac{x^2}{[A^-]}$$

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

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

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

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



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

Create an ICE table

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

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

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

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

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

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

7. For buffers, use the Henderson-Hasselbalch equation, which is the negative logarithm of the K_a equation.

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

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

It's all about the ratio.

If the ratio is > 1, there is more conjugate base than 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 and the pH is less than $\text{p}K_a$ by the logarithm of the ratio.

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	$= 14 + \log [B]$
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			$= pK_a + \log ([A^-]/[HA])$			$= pK_b + \log ([HB^+]/[B])$
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