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.

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

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

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

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

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

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

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

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

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

   Create an ICE table

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

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

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

   $K_a = x^2 / [HA]$

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

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

4. This also works for weak bases.

   $B_{(aq)} + H_2O_{(l)} \rightarrow OH^-_{(aq)} + BH^+_{(aq)}$
   $K_b = [OH^-]\,[BH^+] / [B]$

   Create an ICE table

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

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

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

   $K_b = x^2 / [B]$

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

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

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

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

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

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

   Create an ICE table

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

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

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

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

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

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

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

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

   $BH^+_{(aq)} + H_2O_{(l)} \rightarrow B_{(aq)} + H_3O^+_{(aq)}$

   $K_a = [B]\,[H_3O^+] / [BH^+]$

   Create an ICE table

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

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

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

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

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

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

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

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

   $pOH = pK_b + \log ([HB^+]/[B])$

   It's all about the ratio.

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

Type	K_a	pK_a	pH	K_b	pK_b	pOH
Strong acid	$\geq 1x10^{0}$	≤1	= - log [HA]	$\leq 1x10^{-14}$	≥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	$\leq 1x10^{-14}$	≥14	= 14 + log [B]	$\geq 1x10^{0}$	≤1	= - log [B]

Rev. B – Corrected errors in Henderson-Hasselbalch formula for base