BASIC SKILLS

HOW TO WORK WITH UNITS

All numerical data has units. In chemistry, we use metric “SI” units.

• Convert to SI units.

PICTALF: If the unit is wrong, the answer is wrong!

1. Unit prefixes: Denote powers of “10”
   - 1 cm = 10 mm
   - 1 km = 1000 m

2. Fundamental Units
   - Mass: kilogram (kg)
   - Length: meter (m)
   - Temperature: Kelvin (K)
   - Time: second (s)
   - Amount of a substance: mole
   - Electric charge: coulomb (C)

3. Derived Units
   - Area: length squared, m²
   - Volume: length cubed, m³; 1 liter (L) = 1 dm³
   - Density: mass/volume; common unit kg/m³
   - Speed: distance/time; common unit m/s
   - Electric current: ampere (A) = 1 C/s
   - Force: Newton (N) = 1 kg m/s²
   - Energy: Joule (J) = 1 kg m²/s²
   - Pressure: Pascal (Pa) = 1 kg/(m s²)

4. Fundamental Constants
   - Electron charge, e: 1.602 x 10⁻¹⁹ C
   - Proton charge, e⁺: 1.602 x 10⁻¹⁹ C
   - Mass of electron, mₑ: 9.109 x 10⁻³¹ kg
   - Mass of proton, mₚ: 1.672 x 10⁻²⁷ kg
   - Speed of light, c: 2.997 x 10⁸ m/s

MATH REVIEW

HOW TO WORK WITH ALGEBRAIC EQUATIONS

Give equal treatment to each side.

• Add or subtract:
   - Given: x + y = 5, then x = 5 - y

• Multiply or divide:
   - Given: a(x - y) = b(x - y), then a = b

HOW TO WORK WITH SCIENTIFIC NOTATION

The exponent gives the power of 10.

- Sample: 1.00045 x 10⁴
  - 1.00045 x 10⁴
  - 1.00045 x 10⁴
  - 1.00045 x 10⁴

Sample chemical applications:
- Molar volume of gases: 22.4 L/mol
- Molar mass of NaCl: 58.5 g/mol
- Molar volume of liquids: 1 cm³/mol
- Molar volume of solids: 1 cm³/mol
ATOMIC DATA
* Atomic Number: Z = # of protons.
* Atomic Mass Number: A = # of protons + # of neutrons.
* A and Z are integers. The actual particle mass is given in kg or amu (g/mole). The actual mass is close in value to A.

HOW TO CALCULATE NUCLEAR BINDING ENERGY
The nuclear mass does not equal the sum of proton and neutron masses. The mass difference (Δm, kg/mole) due to the nuclear binding energy (ΔE, J):

\[
\Delta E = \Delta m c^2
\]

**Sample**: Calculate the binding energy for He-4.
Given: He-4 has 2 protons and 2 neutrons
Given: Proton particle mass: 2 x 1.00728 amu
Given: Neutron particle mass: 2 x 1.00866 amu
Calculate: Total particle mass = Sum of proton and neutron particle mass = 4.03188 amu
Given: Actual mass of He-4 nucleus: 4.00150 amu
Calculate: \( \Delta m = 4.03188 - 4.00150 = 0.03038 \) amu

Convert to kg: \( \Delta m = 0.03038 \times 1.66054 \times 10^{-27} \) kg/mole
Calculate: \( \Delta E = \Delta m c^2 \\
= 0.03038 \times 10^{-27} \times (3.00 \times 10^8)^2 \) J/mole

**Pitfall**: Watch units of mass; you can work in kg/particle or amu (g/mole). Note: \( J = kg/m^2/s^2 \).

CALCULATING ATOMIC WEIGHT
For an element with two isotopes:
Atomic wt = mass, \( \chi a_1 \) + mass, \( \chi a_2 \)

**Sample**: Calculate the atomic weight for chlorine.
Given: Chlorine has two isotopes

\[
\begin{align*}
\chi_1 & = 35.453 \\
\chi_2 & = 36.965303 \\
\chi & = 35.453 + 2 \times 36.965303 \\
& = 95.2111 g/mole
\end{align*}
\]

**Pitfall**: Use the actual mass of the nucleus, not the number.

HOW TO IDENTIFY SIGNIFICANT FIGURES (sig. figs.)

* Record all certain digits and one uncertain or estimated digit for a measurement.
* Note: A calculator often includes extra digits in a calculation.
* For a multi-step problem, keep 1 or 2 extra digits; then, round off the final answer.

Rules for the # of sig. figs. in the final answer:
* For addition or subtraction: Use the least number of decimal places found in the data.
  **Sample**: 10.102 + 5.03 = 15.13 (2 dec. places).
* For multiplication or division: The final answer should have same # of sig. figs. as the entry with the fewest sig. figs.
  **Sample**: 5.4020 x 4.00 = 21.8 (3 sig. figs).
* Rounding-off data: Round up if the last uncertain digit is 5 or 5 or over; round down if it is 0 or 2 or 3 or 4. If it is 5, the arbitrary convention is to round up if the last certain digit is odd, round down if it is even.
  **Sample**: 0.0805 => 0.08; 0.035 <= 0.04
  0.453 => 0.45; 0.248 <= 0.25

HOW TO CALCULATE PROPERTIES OF ELECTROMAGNETIC RADIATION
Light waves are characterized by wavelength (\( \lambda \), in m), frequency (\( \nu \), in Hertz, s\(^{-1} \)) and the speed of light (c, in m/s).Sh=the energy is carried in photons.

\[
\begin{align*}
\lambda c &= \nu \lambda \\
\nu &= \frac{c}{\lambda}
\end{align*}
\]

**Sample**: Calculate the \( \nu \) and energy for \( \lambda \) of 500 nm.
Given: \( \lambda = 500 \) nm and \( 1 \) nm = \( 1 \times 10^{-9} \) m
Convert \( \lambda \) to m: \( \lambda = 500 \text{ nm} = 5.00 \times 10^{-7} \) m
Calculate: \( \nu = c/\lambda = 3.00 \times 10^{8} \text{ m/s} / 5.00 \times 10^{-7} \text{ m} \\
= 6.00 \times 10^{14} \text{ s}^{-1} \text{ (Hertz)}
\]
Calculate: energy = \( h \nu \\
= 6.626 \times 10^{-34} \text{ J s} \times 6.00 \times 10^{14} \text{ s}^{-1} \\
= 3.98 \times 10^{-19} \text{ J (s cancels)}
\]

**Pitfall**: The unit on \( \lambda \) should match the unit of c.
HOW TO USE BALANCED EQUATIONS

Sample: 2 Mg + O_2 \rightarrow 2 MgO.

2 Mg atoms and 2 O atoms on each side

2 moles of Mg and 2 moles of O on each side

Calculate the masses of the product and reactants:

Given: A balanced equation and atomic weights: Mg = 24.31; O = 16.00.

Calculate: Mass of Mg = 2 x 24.31 g = 48.62 g of Mg.

Calculate: Mass of O_2 = 2 x 16.00 g = 32.00 g of O_2.

Calculate: Mass of MgO = 2 x 24.31 g + 2 x 16.00 g = 80.62 g of MgO.

Balanced equation conserves mass; 80.62 g on each side.

HOW TO BALANCE AN EQUATION

First: Identify each element in the reaction.

Next: Determine the net charge on each side; this must be balanced in the final equation.

Guidelines: Start with the element found in one compound on each side. Identify compounds that must have the same coefficient. If an element appears in a pure form, leave it to the last step.

You should always check your work!

Pitfall: Coefficients apply to each atom in a molecule or polyatomic ion. You can change coefficients in the equation, not the formula subscripts.

Sample: 2 CH_4 + 3 O_2 \rightarrow 2 CO_2 + 2 H_2 O

First: Elements: C, H, O.

Next: No charge to worry about.

1. H is in CH_4 and H_2O; start with H.

2. The H_2O coefficient must by twice the CH_4 coefficient to balance “H.”

   • 1 CH_4 + 3 O_2 \rightarrow 2 CO_2 + 2 H_2O

   • CH_4 and CO_2 must have the same coefficient.

   • 1 CH_4 + 2 O_2 \rightarrow 1 CO_2 + 2 H_2O

4. Now, determine the O_2 coefficient:

   • 1 CH_4 + 2 O_2 \rightarrow 1 CO_2 + 2 H_2O

5. Check your work: 1 C, 4 H and 4 O on each side...It is balanced!

BALANCING A REDOX EQUATION USING THE HALF-REACTION METHOD

• Split the reaction into oxidation and reduction half-reactions.

• You may need to add H_2O and H^+ for acidic, or H_2O and OH^- for basic reaction conditions.

• Balance these separately, then combine to balance the exchange of electrons.

Sample: Balanced following the acidic solution:

MnO_4^- + Fe^{2+} \rightarrow Mn^{2+} + Fe^{3+}.

1. In acidic solution: Add H^+ to the left and H_2O to the right side:

   MnO_4^- + Fe^{2+} + H^+ \rightarrow H_2O + Mn^{2+} + Fe^{3+}.

2. Identify the half-reactions:

   Fe^{2+} \rightarrow Fe^{3+} (oxidation)

   MnO_4^- + H^+ \rightarrow Mn^{2+} + H_2O (reduction)

3. Add electrons to account for valence changes:

   Fe^{2+} \rightarrow Fe^{3+} + e^-

   Fe(II) \rightarrow Fe(III)

   5e^- + MnO_4^- + H^+ \rightarrow Mn^{2+} + H_2O

4. Balance each half-reaction:

   a. Oxidation: Multiply by a factor of 5 to match electrons in reduction step:

      5 Fe^{2+} \rightarrow 5 Fe^{3+} + 5 e^-

      Charge: +10 on each side, balanced!

   b. Reduction: Balance O, then H^+:

      check charge: 5e^- + MnO_4^- + 8 H^+ \rightarrow Mn^{2+} + 4 H_2O + 5 Fe^{3+}

      Charge: +2 on each side, balanced!

   5. Combine half-reactions to eliminate the 5e^-:

      5 Fe^{2+} + MnO_4^- + 8 H^+ \rightarrow Mn^{2+} + 4 H_2O + 5 Fe^{3+}

   Check your work: 5 Fe, 1 Mn, 4 O and 8 H on each side, atoms are balanced!

   Charge: +17 on each side, charge is balanced!

Pitfall: Make sure you use the H_2O, H^+ (for acidic), or OH^- (for basic), with the correct half-reaction.

HOW TO CALCULATE THE THEORETICAL YIELD

Mass of a reactant is used to determine mass of product.

Given: Mass of reactant, balanced equation, molar masses of reactants and products

Calculate: Moles of reactant = \text{reactant mass}/\text{reactant molar mass}

Calculate: Molar ratio = \text{product molar mass}/\text{product mass}

Calculate: Moles of product = moles of product x molar ratio

Sample: \text{MgO} produced by burning 10.0g of Mg in excess oxygen.

Balanced equation: 2 Mg + O_2 \rightarrow 2 MgO.

Given: 10.0 g of Mg, Mg at.wt. = 24.305 g.

MgO molar mass = 40.305 g

Calculate: Moles of Mg = 10.0g of Mg/24.305g/mole Mg = 0.411 moles of Mg

Calculate: Molar ratio = 2/1

Calculate: Moles of MgO = 0.411 moles Mg x 1 mole MgO/mole Mg = 0.411 moles of MgO

Calculate: Mass of MgO = 0.411 moles MgO x 40.305 g/mole MgO = 16.6 g MgO

The calculation can also be performed as a single sequence of calculations:

10.0g Mg x 1 mol Mg x 1 mol MgO x 40.305 g MgO = 16.6 MgO

Pitfall: If your balanced equation is wrong, your theoretical yield will usually be wrong.

HOW TO CALCULATE A LIMITING REAGENT FOR 2 REACTANTS

In a reaction with 2 reactants, the mass of product is constrained by the reactant in shortest supply, the limiting reagent.

Given: Balanced equation, mass of reactants, molar masses of reactants; specify reactant #s.

Calculate: Moles of each reactant = mass/molar mass

Calculate: Ideal reactant molar ratio = coefficient of reactant #1/coefficient of reactant #2

Calculate: Actual reactant molar ratio = moles of reactant #1/moles of reactant #2

Determine the limiting reagent:

• If actual reactant molar ratio ≤ ideal reactant molar ratio, then reactant #1 is the limiting reagent.

• If actual reactant molar ratio > ideal reactant molar ratio, then reactant #2 is the limiting reagent.

Calculate the theoretical yield based on the mass of the limiting reagent.

Hint: The limiting reagent is arbitrary, but you must stick with your choice for the entire calculation.

Sample: 10.0g Mg reacts with 10.0g O_2; how much MgO is produced?

Balanced equation: 2 Mg + O_2 \rightarrow 2 MgO.

Given: Mg molar mass = 24.350g; Reactant #1 O_2 molar mass = 32.00g; Reactant #2

Calculate: Moles of Mg = 10.0g Mg/24.350g Mg/mol Mg = 0.411 mol Mg

Calculate: Moles of O_2 = 10.0g O_2/32.00g O_2/mol O_2 = 0.3125 mol O_2

Calculate: Ideal reactant molar ratio = 2/1 = 2

Calculate: Actual reactant molar ratio = moles of Mg/moles O_2 = 0.411/0.3125 = 1.31

Determine limiting reagent: 1.31 is less than 2.0, therefore, Mg is the limiting reagent.

Calculate the yield of MgO based on 10.0 grams of Mg (shown in the previous section).

Pitfall: Make sure you distinguish between the ideal and actual molar ratios.
HOW TO USE THE IDEAL GAS LAW

**MOLES OF A GAS SAMPLE**
- **Given:** T = 300 K; P = 2.5 atm; V = 10.5 L
- **Calculate:** n = \( \frac{PV}{RT} \)
  \[ n = \frac{(2.5 \text{ atm})(10.5 \text{ L})}{(0.082057 \text{ L atm/mol K})(300 \text{ K})} \approx 10.0 \text{ mol} \]

**CALCULATING THE # OF MOLES OF A GAS MOLECULE**
- **Given:** M = 18 g/mol; V = 2.0 L
- **Calculate:** n = \( \frac{PV}{RT} \)
  \[ n = \frac{(1.0 \text{ atm})(2.0 \text{ L})}{(0.082057 \text{ L atm/mol K})(298 \text{ K})} \approx 0.0105 \text{ mol} \]

**CALCULATING THE SPEED OF A GAS MOLECULE**
- **Given:** M = 44 g/mol; V = 30.0 L
- **Calculate:** \( v_{\text{rms}} = \sqrt{\frac{3RT}{M}} \)
  \[ v_{\text{rms}} = \sqrt{\frac{3(0.082057 \text{ atm L/mol K})(298 \text{ K})}{44 \text{ g/mol}}} \approx 500 \text{ m/s} \]

**HOW TO USE GRAHAM'S LAW OF EFFUSION**
- **Given:** M_1 = 28 g/mol; M_2 = 23 g/mol
- **Calculate:** \( \frac{v_1}{v_2} = \sqrt{\frac{M_2}{M_1}} \)
  \[ \frac{v_1}{v_2} = \sqrt{\frac{28 \text{ g/mol}}{23 \text{ g/mol}}} \approx 1.06 \]

**HOW TO USE CHARLES’ LAW**
- **Given:** T_1 = 25°C; T_2 = 50°C
- **Calculate:** \( \frac{V_1}{V_2} = \frac{T_1}{T_2} \)
  \[ \frac{V_1}{V_2} = \frac{273}{50} \approx 5.45 \text{ atm} \]

**HOW TO USE BOYLE’S LAW**
- **Given:** P_1 = 1.0 atm; V_1 = 2.0 L
- **Calculate:** P_2 = \( \frac{P_1V_1}{V_2} \)
  \[ P_2 = \frac{(1.0 \text{ atm})(2.0 \text{ L})}{1.0 \text{ L}} = 2.0 \text{ atm} \]

**HOW TO USE THE AVOGADO’ S LAW**
- **Given:** M = 2.0 moles/L; V = 3.0 L
- **Calculate:** \( \frac{V}{n} = \frac{R}{M} \)
  \[ \frac{V}{n} = \frac{8.3145 \text{ J/mole K}}{2.0 \text{ moles/L}} \approx 4.2 \text{ L/mole} \]

**SOLIDS & LIQUIDS**

**HOW TO CALCULATE THE DENSITY OF A SOLID**
- **Given:** Mass = 5.0 g; Volume = 10.0 cm^3
- **Calculate:** Density = \( \frac{\text{mass}}{\text{volume}} \)
  \[ \text{Density} = \frac{5.0 \text{ g}}{10.0 \text{ cm}^3} = 0.5 \text{ g/cm}^3 \]

**HOW TO CALCULATE THE MOLAR MASS OF A SOLID**
- **Given:** Mass = 5.0 g
- **Calculate:** Molar Mass = \( \frac{\text{mass}}{\text{moles}} \)
  \[ \text{Molar Mass} = \frac{5.0 \text{ g}}{0.096 \text{ moles}} \approx 52 \text{ g/mol} \]

**HOW TO CALCULATE THE DENSITY OF A LIQUID**
- **Given:** Mass = 5.0 g; Volume = 10.0 cm^3
- **Calculate:** Density = \( \frac{\text{mass}}{\text{volume}} \)
  \[ \text{Density} = \frac{5.0 \text{ g}}{10.0 \text{ cm}^3} = 0.5 \text{ g/cm}^3 \]

**HOW TO CALCULATE THE MOLAR MASS OF A LIQUID**
- **Given:** Mass = 5.0 g; Volume = 10.0 cm^3
- **Calculate:** Molar Mass = \( \frac{\text{mass}}{\text{moles}} \)
  \[ \text{Molar Mass} = \frac{5.0 \text{ g}}{0.096 \text{ moles}} \approx 52 \text{ g/mol} \]

**THERMODYNAMICS: HEAT, DISORDER & EQUILIBRIUM**

**THERMAL EXPANSION**
- **Given:** Initial length = 2.0 cm; Final length = 2.5 cm
- **Calculate:** \( \Delta L = L_f - L_i \)
  \[ \Delta L = 2.5 \text{ cm} - 2.0 \text{ cm} = 0.5 \text{ cm} \]

**CONDUCTIVITY**
- **Given:** Density = 1.2 g/cm^3; Thermal conductivity = 0.5 W/mK
- **Calculate:** Thermal conductivity = \( \frac{\text{heat flux}}{\text{temperature gradient}} \)
  \[ \text{Thermal Conductivity} = \frac{0.5 \text{ W/mK}}{1.2 \text{ g/cm}^3} \approx 0.42 \text{ W/mK} \]

**HEAT CAPACITY**
- **Given:** Mass = 5.0 g; Heat capacity = 0.8 J/gK
- **Calculate:** Heat capacity = \( \frac{\text{heat}}{\text{temperature change}} \)
  \[ \text{Heat Capacity} = \frac{0.8 \text{ J/gK}}{5.0 \text{ g}} = 0.16 \text{ KJ/gK} \]

**ENTROPY**
- **Given:** Temperature = 298 K; Entropy change = 0.5 J/K
- **Calculate:** Entropy change = \( \frac{\text{heat}}{\text{temperature}} \)
  \[ \text{Entropy Change} = \frac{0.5 \text{ J/K}}{298 \text{ K}} \approx 0.0016 \text{ KJ/K} \]
THERMODYNAMICS cont.

Calculate: $\Delta H = \text{sum of product } \Delta H_{products}$
- sum of reactant $\Delta H_{reactants}$
Calculate: $\Delta S = \text{sum of product } S^0$
- sum of reactant $S^0$

**Sample:** Calculate DH for the reaction:
$CH_4(g) + O_2(g) = CO_2(g) + 2H_2O(l)$
Given: $\Delta H_{products} = -74.6 \times 2.00 = -393.5 \times 2 = -785.8$.
Calculate: $\Delta H = \text{product } \Delta H_{products} - \text{reactant } \Delta H_{reactants}$
$\Delta H = -393.5 - 571.6 = -890.5$ kJ/mole.
Note: Combustion is an exothermic reaction.

**Sample:** Calculate $\Delta S$ for the phase change:
$H_2O(l) \leftrightarrow H_2O(g)$
Given: $S^0 = 70.0$ 
Calculate: $\Delta S = 188.8 = 118.8 J/k mole (K)$
Note: A gas has more entropy than a liquid.

1. Does the reaction release or absorb heat?
   Examine DH.
   - Exothermic (releases heat): $\Delta H < 0$
   - Endothermic (absorbs heat): $\Delta H > 0$

2. Does the reaction proceed to completion? Is the reaction spontaneous? Examine $\Delta G$.
   - $\Delta G > 0$ not spontaneous $K_{eq} < 1$
   - $\Delta G < 0$ spontaneous $K_{eq} > 1$
   - Use $\Delta G$ to calculate $K_{eq}$

HOW TO CALCULATE $K_{eq}$

**Sample:** Calculate $K_{eq}$ if the $\Delta G$ of a reaction is
-10 kJ/mole at 25°C.
Given: $\Delta G = -10.0 kJ$.
T = 25°C;
R = 8.3145 J/K mole
Calculate: $T(K) = 25 + 273.15 = 298.15 K$
Calculate: $\Delta G = -10.0 J / 1.000 J K^{-1} / -10.0 J K^{-1}$
Calculate: $K_{eq} = e^{-\Delta G / RT}$

$m=x - 0.56$
The equilibrium shifts to the right, a spontaneous reaction.

**Pitfall:** T must be in K; make sure you are consistent with T and kJ.

HOW TO HANDLE THE "ADDITION" OF REACTIONS

1. Hess’ Law: If you “sum” reactions, you also sum $\Delta H$, $\Delta G$, and $\Delta S$.

**Sample:** Calculate AH for the reaction A + B => F
Given: A + B => C
$\Delta H = 50 kJ/mole$
Given: C + D => B + F
$\Delta H = 43 kJ/mole$
Sum of the reactions gives A + D => F
Calculate: $\Delta H = 50kJ/mole + 43kJ/mole = 93kJ/mole$

2. What happens if you reverse a reaction?
If you reverse the reaction, change the sign of DH, AG, or GS.

**Sample:** Determine DH for the reaction C => A + B.
Given: A + B => C
$\Delta H = 50 kJ/mole$
For C => A + B, the reverse of this reaction
Calculate: $\Delta H = -50 kJ/mole$

3. How do equation coefficients impact the DH, $\Delta G$, or $\Delta S$?
Thermodynamic properties scale with the coefficients.

**Sample:** Determine DH for the reaction:
2A + 2C => 2D.
Given: A + C => D
$\Delta H = -50 kJ$
For 2A + 2C => 2D, “double” this reaction.
Calculate: $\Delta H = 2 \times -50 kJ = -100 kJ$.

ACID-BASE CHEMISTRY cont.

For simplicity: $[H_2O]^+ = [H^+]$; [ ] refers to M, molarity; HAc: acetic acid; Ac-: acetate

WHY WATER DISSOCIATES

$H_2O \leftrightarrow OH^- + H^+

- $K_w = [OH^-][H^+]] = 10^{-14}$ at 25°C
- For pure water: $[OH^-] = [H^+] = 1 \times 10^{-7}$ M
- Acidic solution: $[H^+] > 1 \times 10^{-7}$ M
- Basic solution: $[OH^-] < 1 \times 10^{-7}$ M

HOW TO CALCULATE pH & $[H^+]$

**Sample:** Determine the pH for a specific [H+].
Given: $[H^+] = 1.4 \times 10^{-5}$ M
Calculate: $pH = -\log_{10}(1.4 \times 10^{-5}) = 4.85$

**Sample:** Determine pH from pOH.
Given: $pH = 8.5$
Calculate: $[H^+] = 10^{-8.5} = 3.2 \times 10^{-6}$ M

HOW TO CALCULATE pH & [OH^-]

**Sample:** Determine the [OH^-] from pOH or pH.
Given: $pH = 4.5$
Calculate: $[OH^-] = 10^{-4.5} = 9.5$
Calculate: $[HAc] = 10^{-9.5} = 3.2 \times 10^{-10}$ M

HOW TO WORK WITH $K_a$ & $K_b$

1. Acid $HA \leftrightarrow H^+ + A^-$
   $K_a = [H^+][A^-]/[HA]
   - $A^-$: Conjugate base; $K_a(A^-) = K_w/K_a(HA)$
   - $pK_a = -\log_{10}(K_a)$

2. Base $B + H_2O \leftrightarrow BH^+ + OH^-
   $K_b = [BH^+][OH^-]/[B]
   - BH+: Conjugate acid; $K_b(BH^+) = K_a(B)$
   - $pK_b = -\log_{10}(K_b)$; weak bases have large pKb

CALCULATING $K_a$ & $pK_b$ OF CONJUGATE BASE (A) OF AN ACID HA

$K_a(A^-) = K_a/K_b(K_A)$

**Sample:** Determine $K_b$ and $pK_b$ of the conjugate base (A) of an acid HA.

$pK_a = -\log_{10}(K_a)$

**Sample:** Determine $K_b$ and $pK_b$ for the acetate ion, $Ac^-$

**Sample:** Determine $K_a$ from $pK_a$ and $K_b$ for the acetate ion, $Ac^-$

**Sample:** Identify the acid: Acetic acid
Given: $K_a(HAc) = 1.7 \times 10^{-5}$
Calculate: $K_b(Ac^-) = K_w/K_a(HAc)$
$= 1 \times 10^{-14} \times 1.7 \times 10^{-5} = 5.9 \times 10^{-10}$
Calculate: $pK_b(Ac^-) = -\log_{10}(5.9 \times 10^{-10}) = 9.23$

ACID-BASE CHEMISTRY cont.

HOW TO CALCULATE $[H^+]_{eq}$

**Sample:** Determine the $[H^+]_{eq}$ for a 0.40 M NaAc solution.
Step 1: $NaAc$ is a basic salt
Step 2: $Ac^-$ is the base; $K_a(AC^-) = K_w/K_b(KAc)$
$= 5.9 \times 10^{-10}$
Step 3: Solve as a “weak-base dissociation” problem
$[B]_{eq} = 0.40 M Ac^-$; calculate $[OH^-]_{eq}$

**Pitfall:** You must correctly identify the acid or base formed by the salt ions, and determine the $K_b$ or $K_a$.
Acid-Base Chemistry Cont.

How to Calculate pH of a Buffer

Buffer of Weak Acid and Conjugate Base

Start with both weak acid, [HA]_{init}, and salt, [A^-]_{init}.

The equilibrium concentrations are governed by:

\[ K_a = \frac{[H^+]_eq[A^-]_eq}{[HA]_eq} \]

**HA \rightleftharpoons H^+ + A^-**

**Init** \[ [HA]_{init} \] \[ [A^-]_{init} \]

\[ K_0 = a \times [A^-]_{init} + a \times [HA]_{init} \]

Method: Substitute the “equiv” expressions into \( K_0 \) and solve the quadratic equation:

\[ \begin{align*}
  K_0 &= a 	imes [A^-]_{init} + a 	imes [HA]_{init} \\
  &= a^2 + a 	imes ([K_a]_{init} - K_a \times [HA]_{init}) \\
  \text{Given:} & \quad [K_a]_{init} \text{ and } [HA]_{init} \text{. Solve for the roots of the quadratic, } [H^+]_{eq} = \frac{a}{a^2}.
\end{align*} \]

**Sample**: Determine the pH of a buffer of 0.5 M HAc and 0.3 M Ac^-.

**Henderson-Hasselbalch**: 

**pH = pK_a + \log_{10} \left( \frac{[A^-]_{init}}{[HA]_{init}} \right) **

**Sample**: Examine previous buffer problem:

\[ [A^-] = [Ac^-] = 0.3 \text{ M}, \quad [HA] = [HAc] = 0.5 \text{ M} \]

**pK_a = pK_a(HAc) = \log_{10} \left( \frac{[HAc]}{[A^-]} \right) = 4.77**

**pH = 4.77 + \log_{10} \left( \frac{0.3}{0.5} \right) = 4.77 - 0.22 = 4.55**

The approximation works.

How to Do an Acid-Base Titration

A systematic acid-base neutralization used to determine the concentration of an unknown acid or base. At the equivalence point, moles of acid = moles of base.

**Sample**: The titration of 50.00 mL of an HCl solution requires 25.00 mL of 1.00 M NaOH.

**Calculate** [HCl]_{init}:

\[ \text{Equation: } HCl + NaOH \rightarrow NaCl + H_2O \]

**Calculate** [HCl]_{eq}:

\[ \text{Compute: } M(HCl) = mmoles HCl = mmoles NaOH. \]

\[ [HCl]_{eq} = \frac{1:1 \text{ molar ratio of } HCl: NaOH.} \]

**Pitfall**: Watch out for round-off error; take the root of the quotient.

Examination of Chemical Equilibrium

How to Determine if the Reaction is at Equilibrium

**Compare Q_c with K_c**

**Sample**: For the reaction: \( A \rightleftharpoons C \), \( K_c = 0.60 \), the observed \( [A] = 0.1 \text{ and } [C] = 0.20 \).

Is the reaction at equilibrium? If not, predict the shift.

1. \( Q_c = [C]/[A] = 0.20 > 0.60 \). \( K_c \) is not at equilibrium, it will shift to the left.

How to Predict Equilibrium Concentrations

**Sample**: Calculate the equilibrium concentrations for the following gas-phase reaction data:

\[ K_c = 0.64 \cdot [CO]_{init} = [H_2O]_{init} = 0.5 \text{ M} \]

**CO(g) + H_2O(g) \rightleftharpoons CO_2(g) + H_2(g)**

**Init** \[ [CO]_{init} \] \[ [H_2O]_{init} \] \[ 0 \] \[ 0 \]

**Equil** \[ [CO]_{eq} \] \[ [H_2O]_{eq} \] \[ a \] \[ a \]

**Note**: The change “a” is the same for each because of the 1:1:1:1 coefficients in the equation.

Equil \[ [HA] = 0.222 \text{ M} \]

**Check your work**: \( K_c = [CO]_{eq} [H_2O]_{eq} /[CO_2]_{eq} [H_2]_{eq} = 0.64 = a^2/(0.50 - a)(0.50 - a) \)

**Pitfall**: Take square root of each side:

\[ \begin{align*}
  a &= \sqrt{0.50} - (0.50 - a) \\
  &= 0.222 \text{ or } a = -1.2.
\end{align*} \]

Use the first option, since “a” must be positive.

**[CO]_{eq} = [H_2O]_{eq} = 0.222 \text{ M}**

Use \( K_c = [CO]_{eq}/[HCl]_{eq} = 0.64 = a^2/(0.50 - a)(0.50 - a) \)

Check your work:

\[ K_c = (0.222^2/0.278^2) = 0.64 \]

Kinetcis & Equilibrium

The goal of a kinetic study is to measure the reaction rate, determine the rate constant, \( k \), the rate law and the activation energy \( (E_a) \).

How to Determine the Rate Law

For \( A \rightleftharpoons B \), the reaction rate is the rate of appearance of product, \( A[B] \text{/time} \); or, rate of loss of reactant: -\( A[\text{A}] \text{/time} \).

**Sample**: How would you characterize the rate of:

\[ \text{CaCO}_3 (s) \rightarrow \text{CaO(s)} + \text{CO}_2(g) \]

Answer: Focus on rate of \( \text{CO}_2 \) production:

\[ \text{Rate} = \frac{\text{d}[\text{CO}_2]}{\text{dt}} \text{/[time]} \]

How to Determine the Reaction Rate

**For \( A \rightleftharpoons B \text{, the reaction rate is the rate of appearance of product, } A[B] \text{/time} ; \text{ or, rate of loss of reactant: } -A[A] \text{/time}.**

\[ \text{Rate law gives the order of the reaction based on the steps in the overall reaction } A + B \rightleftharpoons C. \]

**1. Rate = k[A], for a first-order reaction.**

**2. Rate = k[A]^2, or k[A][B], for a second-order reaction.**

**3. Rate = k[A]^3, for a zero-order reaction.**

**Pitfall**: Equation coefficients describe the balanced overall reaction, not the mechanism and rate law.