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Quick Study® ACADEMIC

# CHEMISTRY EQUATIONS & ANSWERS™

Essential Tool for Chemistry Concepts, Variables & Equations, Including Sample Problems, Common Pitfalls & Helpful Hints

## CONTENTS

**Your success in chemistry depends on your ability to solve numerical problems.**

## BASIC SKILLS

### CALCULATOR SURVIVAL

- Become familiar with your calculator **before** the exam; make sure you can multiply, divide, add, subtract and use all needed functions.
- Calculators never make mistakes; they take your input (intended & accidental) and give an answer.
- Look at the answer; does it make sense?
- Do a quick estimate to check your work.

**Sample:** 4.34 x 7.68/(1.05 x 9.8) is roughly 4 x 8/(1 x 10) or **3.2**; the actual answer: **3.24.**

### HOW TO DO WORD PROBLEMS

- **Read** and evaluate the question **before** you start plugging numbers into the calculator.
- Identify the variables, constants and equations.
- Write out units of the variables and constants.
- Work out the unit before the number.
- You may have extra information, or you may need to obtain constants from your text.

### HOW TO WORK WITH UNITS

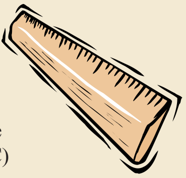
**All numerical data has units. In chemistry, we use metric "SI" units.**

**Pitfall:** If the unit is wrong, the answer is wrong!

1. **Unit prefixes: Denote powers of "10"**

tera T $10^{12}$    giga G $10^{9}$    mega M $10^{6}$
kilo k $10^{3}$    deci d $10^{-1}$    centi c $10^{-2}$
milli m $10^{-3}$    micro µ $10^{-6}$    nano n $10^{-9}$
pico p $10^{-12}$    femto f $10^{-15}$

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, $m^2$
   - **Volume**: length cubed, $m^3$; 1 liter (L) = 1 $dm^3$
   - **Density**: mass/volume; common unit $kg/m^3$
   - **Speed**: distance/time; common unit m/s
   - **Electric current**: ampere (A) = 1 C/s
   - **Force**: Newton (N) = 1 kg $m/s^2$
   - **Energy**: Joule (J) = 1 kg $m^2/s^2$
   - **Pressure**: Pascal (Pa) = 1 kg/(m $s^2$)
4. **Fundamental Constants**

| **Mass** | **in amu (g/mole)** | **in kg** |
|---|---|---|
| electron: | $5.486 \times 10^{-4}$ | $9.10939 \times 10^{-31}$ |
| proton: | 1.007276 | $1.67262 \times 10^{-27}$ |
| neutron: | 1.008664 | $1.67493 \times 10^{-27}$ |

**Electronic charge:** $1.6022 \times 10^{-19}$ C
**Avogadro's number, $N_A$:** $6.02214 \times 10^{23}$
**Ideal gas constant, R:**
R, for gas calculation: 0.082 L atm/(K mol)
R, for energy calculation: 8.314510 J/(K mol)
**Faraday Constant, $\mathscr{F}$:** 96,485 C/mol
**Planck's Constant, h:** $6.626 \times 10^{-34}$ J s
**Speed of Light, c:** $2.9979 \times 10^{8}$ m/s

## BASIC SKILLS *cont.*

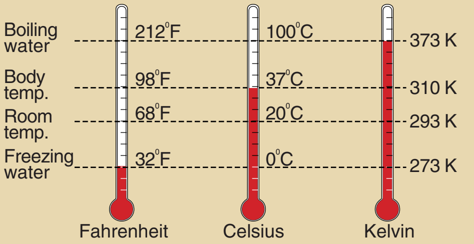
### HOW TO CONVERT DATA

The unit & numerical value are **changed** using a **conversion factor or equation**.

### HOW TO USE EQUATIONS FOR DATA CONVERSION

**Sample:** Convert a temperature of 45˚C to ˚F and Kelvin:
Given: K = ˚C + 273.15
Calculate: Temperature in K = 45˚C + 273.15
= 318.15 K
Given: ˚F = 9/5 ˚C + 32
Calculate: Temperature in ˚F = 9/5 x 45 ˚C + 32
= 81 + 32 = 113 ˚F

T (K) = T (˚C) + 273.15    T (˚F) = 9/5 x T (˚C) + 32



### HOW TO USE A CONVERSION FACTOR

**Sample:** "1 hour = 60 minutes" gives two conversion factors:
1. Multiply by "1 hour/60 minutes" to convert minutes to hours.
2. Multiply by "60 minutes/1 hour" to convert hours to minutes.

**Sample:** Determine the number of hours in 45 minutes.
Given: Conversion factor is "1hour/60 minutes."
Calculate: Time = 45 minutes x (1 hour/60 minutes)
= 0.75 hour (minutes cancel).

**Common conversions:**
1 calorie = 4.184 J    1 kg = 2.2 lb    1 m = 1.1 yd
1 qt = 0.9464 L    1 angstrom (Å) = 1 x $10^{-10}$ m
1 atm = 1.01325 x $10^{5}$ Pa    1 atm = 760 mm Hg

**Pitfall:** Equations and conversion factors have units. Beware of inverting conversion factors.

## MATH REVIEW

### HOW TO WORK WITH ALGEBRAIC EQUATIONS

**Give equal treatment to each side.**

- **Add** or **subtract**:

**Sample:** Given, x = y, then, 4 + x = 4 + y.

- **Multiply** or **divide**:

**Sample:** Given, x = y, then, 4x = 4y and x/5 = y/5.
Given: a = b + 4, then a/(x - 2) = (b + 4)/(x - 2), x ≠ 2.

**Pitfall:** Dividing by zero is not allowed.

### HOW TO WORK WITH SCIENTIFIC NOTATION

**The exponent gives the power of 10.**

**Sample:** 0.00045 = 4.5 x $10^{-4}$; 1345 = 1.345 x $10^{3}$

**Sample chemical applications**: Molecule diameters are $10^{-10}$ m; 1 liter of water contains about 1 x $10^{26}$ atoms.

## MATH REVIEW *cont.*

### HOW TO USE LOGARITHMS & EXPONENTS

- **Common logarithm**, $\log_{10}$: base "10."
  Denotes number or function in powers of 10.
  **Sample:** Given, y = $10^{6}$, then $\log_{10}$ y = 6.
- **Natural logarithm**, ln: base "e"(e = 2.718281829).
  Denotes number or function in powers of "e."
  **Sample:** Given, z = $e^{5}$, then ln z = 5.
- **Products**: log (xy) = log x + log y
- **Powers**: log ($x^{n}$) = n log (x)
- **Multiplication**: Add exponents from each term:
  **Sample:** $10^5 \times 10^3 = 10^{(5+3)} = 10^8$.
- **Division**: Subtract denominator exponents from numerator exponents:
  **Sample:** $10^5/10^3 = 10^{(5-3)} = 10^2$.
- **Square root**: $\sqrt{a} = a^{1/2}$
- **Inverse**: $1/x = x^{-1}$

**Pitfall:** Your calculator has separate keys for lnx (base e), logx (base 10), $10^x$ and $e^x$.

**Sample chemical applications:** pH of acid and base.

### HOW TO CALCULATE ROOTS OF A POLYNOMIAL

An equation of the form: $ax^2 + bx + c = 0$ has 2 solutions or roots, given by the **quadratic** formula:

$[-b + \sqrt{(b^2 - 4\,ac)}]/2a$    **Root 1**
$[-b - \sqrt{(b^2 - 4\,ac)}]/2a$    **Root 2**

**Sample:** Determine the roots for the equation: $3x^2 + 4x + 1 = 0$.
Given: a = 3, b = 4, c = 1
Calculate: Root 1 = $[-4 + \sqrt{(4^2 - 4 \times 3 \times 1)}]/(2 \times 3)$
$= [-4 + \sqrt{(16 - 12)}]/6 = (-4 + 2)/6 = -{}^1/_3$
Calculate: Root 2 = $[-4 - \sqrt{(16 - 12)}]/6 = (-4 - 2)/6 = -1$

**Pitfall:** Beware round-off error. Substitute the roots into the equation to verify results.

**Sample chemical applications**: Weak acids, weak bases, buffers, chemical equilibrium.

### HOW TO DETERMINE THE EQUATION OF A LINE

**LINEAR EQUATION: y = mx + b**

m: **slope** of the line; m = Δy/Δx
b: **y-intercept**, the line crosses the y-axis at "b"; $b = y_i - mx_i$

**Sample:** Determine the equation of a line using (x,y) data.

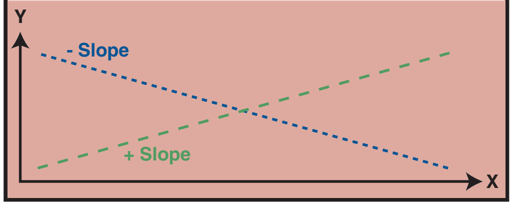
Given:

| | | | | | | |
|---|---|---|---|---|---|---|
| x: | -2 | -1 | 0 | 1 | 2 | 3 |
| y: | -2 | 1 | 4 | 7 | 10 | 13 |

Calculate: Slope = m = Δy/Δx
$= [13 - (-2)]/[3 - (-2)] = {}^{15}/_5 = 3$
Calculate: y-intercept = $b = y_1 - mx_1$
= (-2) - 3 x (-2) = -2 + 6 = 4

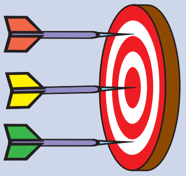
The equation of the line is **y = 3x + 4**.

**Sample chemical applications**: Gas calculations; Beer's Law; analyzing reaction-rate data.



## STATISTICS

### HOW TO CALCULATE EXPERIMENTAL ERROR



- **Accuracy**: The agreement between experimental data and a known value.
- **Error**: A measure of **accuracy**:
  Error = (experiment value - known value).

  Relative error = $\frac{\text{Error}}{\text{known value}}$

  % error = relative error x 100%

  **Sample**: A student finds the mass of an object to be 5.51g; the correct value is 5.80g. What is the % error?

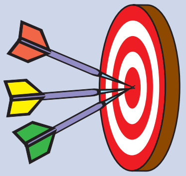
  Given: experimental value = 5.51g;
  known value = 5.80g.

  Calculate: error = (exp. value - known value)
  = 5.51- 5.80g = -0.29g

  Calculate: relative error = error/known value
  = -0.29g/5.8g = - 0.050

  Calculate: % error = relative error x 100%
  = - 0.05 x 100% = - 5.0%

  In this case, we undershoot the known value by 5%.



- **Precision**: The degree to which a set of experimental values agree with each other.

**Pitfall:** A set of data can be precise, but have a large experimental error.

### CALCULATING MEAN & DEVIATION

For a set of numbers, $\{x_1, x_2, x_3 \ldots x_j\}$:

- The **mean,** or average value, is the sum of all "x" divided by "j," the # of entries.
- The deviation, $\Delta_i$, for each $x_i$ is $x_i$ **- mean**; $\Delta_i$ can be positive or negative.

**Sample**: Determine the mean and deviations for the following data: {25, 28, 31, 35, 43, 48}.

Mean = (25 + 28 + 31 + 35 + 43 + 48)/6 = 35

| | | | | | | |
|---|---|---|---|---|---|---|
| $x_i$ | 25 | 28 | 31 | 35 | 43 | 48 |
| $\Delta_i$ | 25 - 35 | 28 - 35 | 31 - 35 | 35 - 35 | 43 - 35 | 48 - 35 |
| $\Delta_i$ | -10 | -7 | -4 | 0 | +8 | +13 |

Note: Sum of $\Delta_i$ = 0.

### 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: 5.46200 x 4.00 = 21.8 (3 sig. figs.).**
- **Rounding-off data**: Round up if the last **uncertain** digit is 6,7,8,9; round down if it is 0,1,2,3,4. If it is a 5: The **arbitrary** convention is to round up if the last **certain** digit is odd, round down if it is even.

  **Sample: 0.085 => 0.08; 0.035 => 0.04**
  **0.453 => 0.45 0.248 => 0.25**

## 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) is 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: Δm = Particle mass - He-4 mass
= 0.03038 amu = 0.03038 g/mole

Convert to kg: $\Delta m = 3.038 \times 10^{-5}$ kg/mole

Calculate: $\mathbf{\Delta E = \Delta mc^2}$
$= 3.038 \times 10^{-5}\text{kg/mole} \times (3.00 \times 10^{8}\text{m/s})^2$
$= 2.73 \times 10^{12}$ 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 = $\text{mass}_a \times \text{fract}_a + \text{mass}_b \times \text{fract}_b$

**Sample**: Calculate the atomic weight for chlorine.

**Given: Chlorine has two isotopes**

| | mass | fractional abundance |
|---|---|---|
| **Cl-35** | **34.968852** | **0.7577** |
| **Cl-37** | **36.965303** | **0.2423** |

Calculate: Atomic wt = $\text{mass}_a \times \text{fract}_a + \text{mass}_b \times \text{fract}_b$
= 34.968853 x 0.7577 + 36.965303 x 0.2423
= 26.496 + 8.9566
= 35.45 amu (4 sig. figs.)

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

### HOW TO CALCULATE PROPERTIES OF ELECTROMAGNETIC RADIATION

Light waves are characterized by **wavelength (λ,** in m), **frequency (υ,** in Hertz, $s^{-1}$**)** and the speed of light (c, in m/s). The energy is carried in **photons.**

$$\lambda\upsilon = c$$

**Energy of a photon = hυ**

**Sample**: Calculate the υ and energy for λ of 500 nm.

Given: λ = 500 nm and 1 nm = $1 \times 10^{-9}$ m

Convert λ to m: λ = 500 nm = $5.00 \times 10^{-7}$ m

Calculate: $\upsilon = c/\lambda = 3.00 \times 10^{8}$ m/s /$5.00 \times 10^{-7}$ m
$= 6.00 \times 10^{14}\ s^{-1}$ (Hertz)

Calculate: energy = hυ
$= 6.626 \times 10^{-34}$ J s x $6.00 \times 10^{14}\ s^{-1}$
$= 3.98 \times 10^{-19}$ J (s cancels)

**Pitfall:** The unit on **λ** should match the unit of **c**.

## CHEMICAL FORMULAS & MOLES

The **formula** and **name** denote elements and relative composition in the compound. A **balanced** equation conserves **atoms** and **moles** of each element.

- One **mole** is Avogadro's number, $N_A$ ($6.023 \times 10^{23}$), of atoms or molecules.
- The **atomic weight**, the mass in grams, of one mole of the atomic element as found in nature, is often given on the Periodic Table, along with the atomic number and element symbol.
- The **molar mass** of a compound is the mass, in grams, of 1 mole of the substance.

### HOW TO CALCULATE MOLAR MASS FROM THE FORMULA

Given: The **atomic weight** (at.wt.) of each element in the compound and the formula coefficients.

Calculate: Molar mass = sum of each element's atomic weight multiplied by the formula **coefficient.**

**Sample**: **Simple case**: $MgCl_2$.

Given: Mg at.wt.: 24.305 g/mole; coefficient = 1
Cl at.wt.: 35.453 g/mole; coefficient = 2

Calculate: Molar mass = 1 x Mg at.wt.+2 x Cl at.wt.
= 1 x 24.305 + 2 x 35.453
= 95.211 g/mole

**Sample**: **Complex case**: $Mg(NO_3)_2 \times 2H_2O$.

Given: Mg at.wt.: 24.305 g/mole; coefficient = 1
N at.wt.: 14.007 g/mole; coefficient = 2
O at.wt.: 15.9994 g/mole; coefficient = 8
H at.wt.: 1.008 g/mole; coefficient = 4

Calculate: Molar mass = 1 x Mg at.wt. + 2 x N at.wt.
+ 8 x O at.wt. + 4 x H at.wt
= 24.305 + 2 x 14.007
+ 8 x 15.9994 + 4 x 1.008
= 24.305 + 28.014
+ 127.9952 + 4.032
= 184.35 g/mole

**Pitfall:** It is easy to miscount the atoms in polyatomic ions or waters of hydration.

### HOW TO CALCULATE ELEMENTAL % COMP

The portion of the mass coming from each element in the compound; the %-comps sum to 100%.

Given: Chemical formula, compound molar mass and atomic weights for each element.

Step 1: Sum the formula coefficients to determine the number of atoms of each element.

Step 2: The mass of each element = at.wt. x number of atoms of that element.

Calculate: % comp for element A = 100% x mass of A/compound molar mass

**Sample**: Determine the elemental % comp of Mg and Cl in $MgCl_2$.

Given: $MgCl_2$, molar mass = 95.21 g/mole;
Mg at.wt. = 24.305 g/mole;
Cl at.wt. = 35.453 g/mole

Step 1: $MgCl_2$ has 1 atom of Mg
$MgCl_2$ has 2 atoms of Cl

Step 2: Mass of Mg = 24.305 g/mole x 1
= 24.305 g/mole
Mass of Cl = 35.453 g/mole x 2
= 70.906 g/mole

Calculate: **Mg % comp**
= 100% x 24.305/95.21
= 25.53% Mg

Calculate: **Cl % comp**
= 100% x 70.906/95.21 = 74.47 %

Sum of elemental % comp
= 25.53% + 74.47% = 100.00%

**Pitfall:** In a complex formula, the same element may exist in different ions.

# CHEMICAL FORMULAS & MOLES *cont.*

## HOW TO CALCULATE THE # OF MOLECULES

Given: **x**, the mass of the sample, and the molar mass of the material

Calculate: Number of moles = $\frac{\text{x (in g)}}{\text{molar mass (g/mole)}}$

Calculate: Number of molecules = # of moles x Avogadro's number ($N_A$)

**Sample**: Determine the number of moles and the number of water molecules in 5.00 grams of water vapor.

Given: 5.00 g of $H_2O$; molar mass = 18.015 g/mole

Calculate: # of moles = 5.00g $H_2O$/18.015g/mole $H_2O$ = 0.278 moles $H_2O$

Calculate: # of molecules = 0.278 moles $H_2O$ x 6.022 x $10^{23}$ molecules/mole = 1.67 x $10^{23}$ $H_2O$ molecules

This could also be determined in a single calculation:
5.00g x 1 mole/18.015g x $N_A$ molecules/mole
= 1.67 x $10^{23}$ molecules

## HOW TO CALCULATE EMPIRICAL FORMULAS

Given: % composition and atomic weights, start by converting "%" to "grams of element"; assume you have 100 g of sample.

Calculate: Moles for each element = grams of element ÷ atomic weight of the element.

Calculate: The formula coefficient for each element = number of moles ÷ the smaller number of moles calculated in the previous step.

To determine the **empirical formula**, multiply each coefficient by a number to give whole # coefficient.

**Sample**: Determine the empirical formula for a compound containing 75% C & 25 % H by mass.

Given: Atomic weights: C at.wt. = 12.011;
H at.wt. = 1.008.
Assume you have 75 g of C and 25 g of H (total mass = 100 g).

Calculate: The number of moles for each element:
75 g of C/12.011g/mole C
= 6.24 moles of C
25g of H/1.008 g/mole H
= 24.8 moles of H.

Calculate: The formula coefficient for each element:
C formula coefficient: 6.24/6.24 = 1.00.
H formula coefficient: 24.8/6.24 = 3.97.
The empirical formula is $CH_4$.

**Pitfall:** Due to experimental error, the calculated formula coefficients may not be integers.

## HOW TO DERIVE THE MOLECULAR FORMULA FROM THE EMPIRICAL FORMULA

The molecular formula coefficients are obtained by multiplying each empirical formula coefficient by a **factor:** The molecular molar mass ÷ empirical molar mass.

Given: The empirical formula, molecular molar mass, and atomic weights.

Calculate: Empirical molar mass = sum of at.wts. in the empirical formula.

Calculate: The molecular ÷ empirical factor = molecular molar mass ÷ empirical molar mass.
Determine the molecular formula by multiplying each empirical coefficient by this factor.

**Sample**: Determine the molecular formula for a compound with molar mass 28 and empirical formula $CH_2$.

Given: The empirical formula is $CH_2$;
C at.wt. =12.0; H at.wt. = 1.0.

Calculate: The empirical molar mass = 12 + 2 = 14.

Calculate: The molecular/empirical factor = 28/14 = 2.
The **molecular** formula is $C_2H_4$; the coefficients are **twice** the **empirical** formula coefficients.

# STOICHIOMETRY

## HOW TO USE BALANCED EQUATIONS

**Sample**: $2 Mg + O_2 => 2 MgO$.

**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 Mg at.wt. = 48.62g of Mg.

Calculate: Mass of $O_2$ = 2 x O at.wt. = 32.00g of $O_2$.

Calculate: Mass of MgO = 2 x Mg at.wt. + 2 x O at.wt. = 80.62g of MgO.

48.62g of Mg reacts with 32.00g of $O_2$ to produce 80.62g of MgO.

Balanced equation conserves mass; 80.62g 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**: $\underline{?}\ CH_4 + \underline{?}\ O_2 => \underline{?}\ CO_2 + \underline{?}\ H_2O$

**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."
   - $1\ CH_4 + \underline{?}\ O_2 => \underline{?}\ CO_2 + 2\ H_2O$
3. $CH_4$ and $CO_2$ must have the same coefficient.
   - $1\ CH_4 + \underline{?}\ O_2 => 1\ CO_2 + 2\ H_2O$
4. Now, determine the $O_2$ coefficient:
   - $1\ CH_4 + 2\ O_2 => 1\ CO_2 + 2\ H_2O$
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**: Balance the following for acidic solution:
$MnO_4^- + Fe^{2+} => Mn^{2+} + Fe^{3+}$.

1. In acidic solution: Add $H^+$ to the left and $H_2O$ to the right side:
   $MnO_4^- + Fe^{2+} + H^+ => H_2O + Mn^{2+} + Fe^{3+}$
2. Identify the half-reactions:
   $Fe^{2+} => Fe^{3+}$ (oxidation)
   $MnO_4^- + H^+ => Mn^{2+} + H_2O$ (reduction)
3. Add electrons to account for valence changes:
   $Fe^{2+} => Fe^{3+} + 1e^-$ Fe(II) to Fe(III)
   $5e^- + MnO_4^- + H^+ => Mn^{2+} + H_2O$ Mn(VII) to Mn(II)
4. Balance each half-reaction:
   a. **Oxidation**: Multiply by a factor of 5 to match electrons in reduction step:
   $5\ Fe^{2+} => 5\ Fe^{+3} + 5\ e^-$
   Charge: +10 on each side, balanced!
   b. **Reduction**: Balance O, then $H^+$;
   check charge: $5e^- + MnO_4^- + 8H^+ => Mn^{2+} + 4H_2O$
   Charge: +2 on each side, balanced!
5. Combine half-reactions to eliminate the $5e^-$:
   $5\ Fe^{2+} + MnO_4^- + 8\ H^+ => Mn^{2+} + 4\ H_2O + 5\ Fe^{3+}$
   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.

# STOICHIOMETRY

## 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 = $\frac{\text{reactant mass}}{\text{reactant molar mass}}$

Calculate: *Molar ratio* = $\frac{\text{product equation coefficient}}{\text{reactant equation coefficient}}$

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

Calculate: Mass of product
= moles of product x product molar mass

**Sample**: Calculate the mass of Mg produced by burning 10.0g of Mg in excess oxygen.
Balanced equation: $2 Mg + O_2 => 2 MgO$

Given: 10.0 grams of Mg, Mg at.wt. = 24.305 g, MgO molar mass = 40.305 g

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

Calculate: Molar ratio = $^2/_2$ = 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 MgO/mole MgO
= 16.6 g MgO

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

$$10.0 \mathit{g\ Mg} \times \frac{1\ \mathit{mol\ Mg}}{24.305 \mathit{g\ Mg}} \times \frac{1\ \mathit{mol\ MgO}}{1\ \mathit{mol\ Mg}} \times \frac{40.35\text{g MgO}}{1\ \mathit{mol\ MgO}}$$

**= 16.6 g MgO (note canceled units in *italics*)**

**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 = $\frac{\text{mass}}{\text{molar mass}}$

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 reactant numbering 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: $2 Mg + O_2 => 2 MgO$

Given: Mg molar mass = 24.305g; Reactant #1
$O_2$ molar mass = 32.00g; Reactant #2

Calculate: Moles of Mg = 10.0g Mg/24.305g Mg/mol Mg = 0.411 mol Mg
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 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.

## WORKING WITH GASES

$$PV = nRT$$

**Ideal Gas Law**

Simple model for gas behavior.

**Pressure**, P; common units: atm, Pa, bar or mm Hg; the R given below is for P in **atm**.

**Volume**, V; common units: liter (L), $m^3$; the R given below is for V in L.

**Temperature**, T; common units: **Kelvin**, °C or °F; always convert °C and °F to Kelvin.

**Number of moles**, n; moles = gas mass/gas molar mass

**Ideal Gas constant** = **R** = 0.082 L atm/(mol K)

⚠ **Pitfall: All** data must fit the units of R.

### HOW TO CALCULATE THE # OF MOLES OF A GAS SAMPLE

Given: Mass of gas (g), molar mass of gas

Calculate: Moles = mass of sample/**molar mass**

**Sample**: Determine # of moles in 5.0g of $H_2$ gas.

Given: 5.0g sample, $H_2$ molar mass = 2.016 g/mole.

Calculate: Moles of $H_2$ = $5.0_g$ $H_2$ x 1 mole. $H_2/2.016_g$ H2 = 2.48 mol $H_2$.

If you are given density and volume, first calculate mass of the gas; mass (g) = ρ(g/L) x V(L).

### HOW TO USE THE IDEAL GAS LAW

**Sample**: Calculate the pressure for 2.5 moles of Ar gas occupying 3.5 liters at 25°C.

Make required changes to variables:

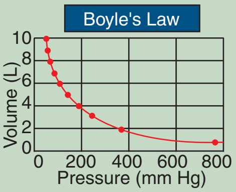
T(K) = 25°C + 273.15 = 298.15K

Calculate: P = nRT/V = 2.5 moles x 0.082L atm/(mol K) x 298.15K/3.5L

**= 17.5 atm (Other units cancel)**

### HOW TO USE BOYLE'S LAW

P & V are inversely proportional with constant T & n.



This is an **inverse-proportionality** problem:

- P α $^1/_V$
  Given: V changes by a factor of z.
  Calculate: $P_{fin} = {}^1/_z$ x Pinit.
- V α $^1/_P$
  Given: P changes by a factor of z.
  Calculate: $V_{fin} = {}^1/_z$ x $V_{init}$

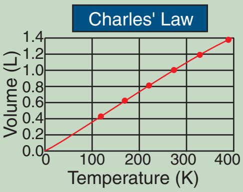
**Sample**: The pressure of a 4.0L sample changes from 2.5 atm to 5.0 atm. What is the final V?

Given: P changes 2-fold: 2.5 to 5.0 atm

Calculate: $V_{fin} = {}^1/_2$ x $V_{init} = {}^1/_2$ x 4.0L = 2.0L

### HOW TO USE CHARLES' LAW

V and T are linearly proportional with constant n & P



This is a **direct-proportionality** problem: V α T:

Given: T changes by a factor of z.

Calculate: $V_{fin}$ = z x $V_{init}$.

⚠ Pitfall: T must be in Kelvin; convert °C to K.

**Sample**: A 3.5L sample of He gas is at 300 K; the T is raised to 900 K; what is the new V?

Given: T increases 3-fold: 300 to 900 K

Calculate: $V_{fin}$ = 3 x $V_{init}$ = 3.0 x 3.5 L = 10.5 L

## WORKING WITH GASES *cont.*

### HOW TO USE AVOGADRO'S LAW

$$V \alpha n$$

V is proportional to n with constant T & P.

This is a **direct-proportionality** problem:

Given: The # of moles changes by a factor of z.

Calculate: $V_{fin}$ = z x $V_{init}$.

**Sample**: A 2.0 mole gas sample occupies 30.0L. Determine V for 1.0 mole of the gas.

Given: n changes by a factor of $^1/_2$

Calculate: $V_{fin}$ = $^1/_2$ x 30.0 L = 15.0 L

### HOW TO CALCULATE THE SPEED OF A GAS MOLECULE

$$v_{rms} = \sqrt{\frac{3RT}{M}}$$

**Note:** R = 8.314510 **J/(K mol)** = 8.314510 **kg m²/(s² K mol)**

**Sample**: Calculate the vrms for He at 300 K

Given: T = 300;

He, M = 4.00 g/mol = 4.00 x10-3 kg/mol

Calculate: $v_{rms} = \sqrt{(3\ RT/\ M)}$

$= \sqrt{(3 \text{ x } 8.31451 \text{ kg m}^2/\text{s}^2/(\text{K mol}) \text{ x } 300 \text{ K}/4.00 \text{ x } 10^{-3} \text{ kg/mol})}$

$= \sqrt{(1.87 \text{ x } 10^6 \text{ m}^2/\text{s}^2)}$ = **1,370 m/s**

⚠ **Pitfall:** Watch the units on R and M; the final unit is m/s. T must be in Kelvin.

### HOW TO USE GRAHAM'S LAW OF EFFUSION

$$\frac{\text{Rate } M_1}{\text{Rate } M_2} = \sqrt{\frac{M_2}{M_1}}$$

The **relative** rate of effusion for molecules of mass $M_1$ and $M_2$

**Sample**: Determine relative rate of effusion for $H_2$ and $CO_2$.

Given: $M_1 = M_{H2} = 2$ g/mol; $M_2 = M_{CO2} = 44$ g/mol

Calculate: Rate $H_2$/Rate $CO_2 = \sqrt{(44/2)} = 4.7$

$H_2$ diffuses 4.7 times as fast as CO2

⚠ Pitfall: It is easy to invert the $M_1/M_2$; the smaller atom is always faster.

## SOLIDS & LIQUIDS

### CALCULATING MOLES OF REAGENTS

Determine the # of **moles** in "x-grams," or the **mass** needed to give a certain # of moles.

Required data: The **molar mass**.

**Sample**: Calculate # of moles in 5.6 g of NaCl.

Given: NaCl molar mass = 58.44 g

Calculate: Moles of NaCl = 5.6g/58.44g/mole = 0.096 moles NaCl

**Sample**: Calculate mass of 0.25 moles of NaCl.

Calculate: Mass of NaCl = 0.25 moles x 58.44g/mole = 14.61g NaCl

### HOW TO CALCULATE MASS OF LIQUIDS

$$\text{vol x } \rho = \text{mass}$$

**Density (ρ)**, has units of g/mL.

**Pure reagent**: Use **ρ** & volume to determine the mass.

**Sample**: Determine the mass of 30.0 mL of methanol.

Given: r = 0.790 g/mL

Calculate: Mass = vol x r = 30.0mL x 0.790 g/mL = 23.7 g

## SOLIDS & LIQUIDS *cont.*

### HOW TO CALCULATE MOLES OF REAGENTS IN SOLUTION

Common units: **Molarity (M)**: Moles of solute **per liter of solution**; **molality (m),** moles of solute **per kg of solvent**. Multiply the solution volume by the molarity to calculate **moles** of reagent.

Given: Solution molarity (M)

Calculate: Moles = vol x M

⚠ **Pitfall:** Volume should be in L. If you want to use "mL," denote M as "mmol/mL of solution"; **mmol = 0.001 mole**.

**Sample**: Determine the moles and mass of NaCl in 25 mL of 2.35 M NaCl solution.

Given: NaCl molarity = 2.35 M; molar mass = 58.44 g

Calculate: Volume = 25 mL x 1 L/1000 mL = 0.025 L

Calculate: NaCl moles = 2.35 mol/L x 0.025 L = 0.059 moles

Calculate: NaCl mass = 0.059 moles x 58.44 g/mole = 3.45 g

### HOW TO PREPARE SOLUTIONS

A **solution** is prepared by dissolving a known mass of solid in a specific amount of solvent.

**Sample**: Prepare **one** liter of 1.00 M NaCl.

Given: NaCl molar mass = 58.44 g/mole

Step 1. Weigh out 58.44 g of NaCl and transfer to a 1 L volumetric flask.

Step 2. Dissolve the salt; fill with water to the 1-L line.

Note: If you need a different M, change the mass of NaCl.

### PREPARING A DILUTE SOLUTION FROM A STOCK SOLUTION

**Key**: Conserve mass and moles. The molarity and volume of the stock and diluted solutions are governed by:

$$M_{stock} \text{ x } V_{stock} = M_{dilute} \text{ x } V_{dilute}$$

**Sample**: Prepare 50 mL of a 1.0 M solution from "a" mL of 2.0 M stock.

Given: $M_{stock}$ = 2.0 M; $V_{stock}$ = a;
$M_{dilute}$ = 1.0 M; $V_{dilute}$ = 50 mL

Calculate: "a" mL = 50mL x 1.0M/2.0M = 25mL

### HOW TO CALCULATE COLLIGATIVE PROPERTIES

One example is **freezing point depression:**

$$\Delta T_f = -\text{ m x } K_f \text{ x ion factor}$$

m: Molality; $K_f$: solvent constant;

Ion factor: # of ions produced by solute: 1 for Molecular solute; 2 or more for ionic salt

**Sample**: Calculate the freezing point depression for a solution of 100g of NaCl in 500g of water.

Given: $K_f$ (water) = 1.86 °C/m;
molar mass of salt = 58.44 g/mol
Ion factor = 2

Calculate: Mass of solvent = 500g x 1kg/1,000g = 0.500 kg

Calculate: m of NaCl = (100.0g/58.44g/mol)/0.500kg = 3.42 m

Calculate: ΔT = - 3.42 m x 1.86 °C/m x 2 = -12.72 °C

## THERMODYNAMICS: HEAT, DISORDER & EQUILIBRIUM

- ΔH (enthalpy), DG (free energy) and DS (entropy) characterize a process.

$$\Delta G = \Delta H - T\ \Delta S \text{ and } \Delta G = -RT \ln K_{eq}$$

### HOW TO CALCULATE ΔG, ΔH, ΔS FROM STANDARD DATA

Given: $\Delta G_f0$ (Free Energy of Formation), in kJ/mole; $\Delta H_f0$ (Enthalpy of Formation), in kJ/mole;
$S^0$ (Standard Entropy), J/(mole K)

Calculate: ΔG = sum of product $\Delta G_f0$ - sum of reactant $\Delta G_f0$

## THERMODYNAMICS *cont.*

Calculate: $\Delta H$ = sum of product $\Delta H_f0$
- sum of reactant $\Delta H_f0$

Calculate: $\Delta S$ = sum of product $S^0$
- sum of reactant $S^0$

**Sample**: Calculate DH for the reaction:
$CH_4(g) + 2O_2(g) \Rightarrow CO_2(g) + 2H_2O(l)$.
Given: $\Delta H_f0$ -74.6 2 x 0.0 -393.5 2 x -285.8.
Calculate: $\Delta H$ = product $\Delta H_f0$ - reactant $\Delta H_f0$.
$\Delta H$ = -393.5 -571.6 +74.6 = -890.5 kJ/mole.
Note: Combustion is an exothemic reaction.

**Sample**: Calculate $\Delta S$ for the phase change:
H2O(l) => H2O(g)
Given: S0 70.0 188.8
Calculate: $\Delta S$ = 188.8 - 70.0 = 118.8 J/(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.

$K_{eq} = e^{-\Delta G/RT}$

Given: $\Delta G$ = -10 kJ;
T = 25°C;
R = 8.3145 J/(K mole)
Calculate: T(K) = 25 °C + 273.15 = 298.15 K
Calculate: $\Delta G$ = -10 kJ x 1,000 J/kJ = -10,000 J
Calculate: $K_{eq}$ = exp (- (-10,000 J/mole)
/(8.3145 J/(K mole) x 298.15 K)
= $_e4.03$ = 56.5

The equilibrium shifts to the right, a **spontaneous reaction.**

Pitfall: T must be in K; make sure you are consistent with J 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 $\Delta H$ for the reaction A + D => 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: DH = 50kJ/mole + 43kJ/mole = 93kJ/mole

**2. What happens if you reverse a reaction?**
If you reverse the reaction, **change the sign** of DH, $\Delta G$ or $\Delta S$.

**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 => 2 D, "double" this reaction.
Calculate: $\Delta H$ = 2 x -50 kJ = -100 kJ.

## ACID-BASE CHEMISTRY

For simplicity: $[H_3O^+] = [H^+]$; [] refers to M, molarity; HAc = acetic acid; $Ac^-$ = acetate

### WHY WATER DISSOCIATES $H_2O \Leftrightarrow OH^- + H^+$

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

### HOW TO CALCULATE pH & [H+]

$pH = -\log_{10}[H^+]$ $[H^+] = 10^{-pH}$

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

**Sample**: Determine $[H^+]$ from pH.
Given: pH = 8.5
Calculate: $[H^+] = 10^{(-8.5)}$ = 3.2 x $10^{-9}$ M

### HOW TO CALCULATE pOH & [OH-]

$pOH = -\log_{10}[OH^-]$ $[OH^-] = 10^{-pOH}$
**pOH + pH = 14 for any given solution**

**Sample**: Determine the $[OH^-]$ from pOH or pH.
Given: pH = 4.5
Calculate: pOH = 14 - 4.5 = 9.5
Calculate: [OH-] = $10^{(-9.5)}$ = 3.2 x $10^{-10}$ M

### HOW TO WORK WITH $K_a$ & $K_b$

**1. Acid** $HA \Leftrightarrow H^+ + A^-$

- $K_a = [H^+]_{eq}[A^-]_{eq}/[HA]_{eq}$
- $A^-$ : Conjugate base; $K_b(A^-) = K_w/K_a(HA)$
- $pK_a = -\log_{10}(K_a)$

**2. Base** $B + H_2O \Leftrightarrow BH^+ + OH^-$

- $K_b = [OH^-]_{eq}[BH^+]_{eq}/[B]_{eq}$
- $BH^+$: Conjugate acid; $K_a(BH^+) = K_w/K_b(B)$
- $pK_b = -\log_{10}(K_b)$; weak bases have large $pK_b$

### CALCULATING $K_a$

Substitute the experimental equilibrium concentrations into the $K_a$ expression.

$$K_a = \frac{[H^+]_{eq}[A^-]_{eq}}{[HA]_{eq}}$$

**Sample**: Determine $K_a$ and $pK_a$ from equilibrium concentration data for HA.
Given: $[H^+]_{eq}$ = 1x$10^{-4}$ M; $[A^-]_{eq}$ = 1x$10^{-4}$ M; $[HA]_{eq}$ = 1.0 M
Calculate: **$K_a$** = 1x$10^{-4}$ x 1x$10^{-4}$/1.0 = 1x$10^{-8}$
Calculate: **$pK_a$** = $-\log_{10}$ (1x$10^{-8}$) = 8.0

### HOW TO CALCULATE $K_b$ & $pK_b$ OF CONJUGATE BASE ($A^-$) OF AN ACID HA

$K_b(A^-) = K_w/K_a(HA)$

**Sample**: Determine $K_b$ and $pK_b$ for the acetate ion, $Ac^-$.
**Identify the acid:** Acetic acid
Given: $K_a$(HAc) = 1.7 x $10^{-5}$
Calculate: **$K_b(Ac^-)$** = $K_w/K_a$(HAc)
= 1x$10^{-14}$/1.7x$10^{-5}$ = 5.9 x $10^{-10}$
Calculate: **$pK_b(Ac^-)$** = $-\log_{10}$(5.9 x $10^{-10}$) = 9.23

### HOW TO CALCULATE % DISSOCIATION OF AN ACID

$$\text{\% dissociation} = 100\% \times \frac{[H^+]_{eq}}{[HA]_{initial}}$$

**Sample**: Determine the % diss. for a 0.50 M HA that produces $[H^+]_{eq}$ = 0.10 M and $[HA]_{eq}$= 0.4.
Given: $[H^+]_{eq}$ = 0.10 M; $[HA]_{initial}$ = 0.50 M
Calculate: **% diss.** = 100% x 0.10/0.50 = 20%

**Pitfall:** Be sure to use $[HA]_{initial}$, not $[HA]_{eq}$.

## ACID-BASE CHEMISTRY *cont.*

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

| | HA | <=> | $H^+$ | + | $A^-$ |
|---|---|---|---|---|---|
| Init | $[HA]_{init}$ | | 0 | | 0 |
| Equil | $[HA]_{init}$-a | | a | | a |

**Method:** Substitute the "Equil" expressions into $K_a$ and solve the quadratic equation:
**Start with:** $K_a = a^2/([HA]_{init} - a)$
This rearranges to: $K_a$ x $([HA]_{init} - a) = a^2$
$a^2 + K_a$ x a - $K_a$ x $[HA]_{init} = 0$
Given $K_a$ and $[HA]_{init}$, use the quadratic formula to obtain "a," $[H^+]_{eq}$.

**Sample**: Calculate $[H^+]$ for 0.5 M HAc.
Given: $K_a$ = 1.7 x 10 - 5
Substitute into quadratic equation:
$a^2 + K_a$ x a - $K_a$ x $[HAc]_{init} = 0$
$a^2$ + 1.7 x $10^{-5}$ x a - 1.7 x $10^{-5}$ x 0.50 = 0
$a^2$ + 1.7 x $10^{-5}$ x a - 8.5 x $10^{-6}$ = 0
Solve the quadratic equation:
a = $[H^+]_{eq}$ = 0.0029 M
**Check your work:** $K_a$ = (0.0029 x 0.0029)
/(0.5 - 0.0029) = 1.7 x $10^{-5}$

**Pitfall:** Watch out for round-off error when you solve for the roots of the quadratic equation.

### HOW TO CALCULATE THE $[OH^-]_{eq}$

| | B | + | $H_2O$ | <=> | $BH^+$ | + | $OH^-$ |
|---|---|---|---|---|---|---|---|
| Init | $[B]_{init}$ | | | | 0 | | 0 |
| Equil | $[B]_{init}$-a | | | | a | | a |

**Method:** Substitute the "Equil" expressions into $K_b$ and solve the quadratic equation:
**Start with**: $K_b = a^2/([B]_{init} - a)$
Solve this quadratic equation for "a" = $[OH^-]_{eq}$

### WHY DO SALTS HYDROLYZE?

**Basic Salts** react with water to form $OH^-$.
**Sample**: Sodium acetate: $Ac^- + H_2O \Leftrightarrow HAc + OH^-$

**Acidic Salts** react with water to form $H_3O^+$.
**Sample:** Ammonium chloride:
$NH_4^+ + H_2O \Leftrightarrow NH_3 + H_3O^+$

**Neutral Salts** do not react with water.
**Sample:** NaCl (product of strong acid + strong base)

### HOW TO CALCULATE THE [H+] OR [OH-] FOR A SALT

Step 1: Is the salt acidic, basic or neutral?
Step 2: If acidic: Identify the weak acid, and the $K_a$; if basic: Identify the weak base, and the $K_b$. If neutral: The solution will not have acidic or basic character.
Step 3: Set up the problem as a weak-base or weak-acid dissociation problem. Given the initial salt concentration, calculate the equilibrium $[H^+]$ or $[OH^-]$.

**Sample**: Determine the $[H^+]$ or $[OH^-]$ for a 0.40 M **NaAc** solution.
Step 1: **NaAc is a basic salt**
Step 2: $Ac^-$ is the base; $K_b(Ac^-) = K_w/K_a(HAc)$ = 5.9 x $10^{-10}$
Step 3: Solve as a "weak-base dissociation" problem $[B]_{init}$ = 0.40 M $Ac^-$; calculate $[OH^-]_{equil}$

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

# 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 $K_a = [H^+]_{eq}[A-]_{eq}/[HA]_{eq}$.

| | HA | <=> | $H^+$ + | $A^-$ |
|---|---|---|---|---|
| **Init** | $[HA]_{init}$ | | 0 | $[A^-]_{init}$ |
| **Equil** | $[HA]_{init}$-a | | a | $[A^-]_{init}$+a |

**Method**: Substitute the "Equil" expressions into $K_a$ and solve the quadratic equation:

$K_a = a \times ([A^-]_{init} + a)/([HA]_{init} - a)$

$K_a \times [HA]_{init} - a \times K_a = a \times [A^-]_{init} + a^2$

$a^2 + a \times (K_a + [A^-]_{init}) - K_a \times [HA]_{init} = 0$

Given: $K_a$, $[A^-]_{init}$ and $[HA]_{init}$, solve for the roots of the quadratic, $a = [H^+]_{eq}$

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

Given: $K_a$ (HAc) = $1.7 \times 10^{-5}$

Quadratic: $0 = a^2 + a \times (1.7 \times 10^{-5} + 0.3)$
$-1.7 \times 10^{-5} \times 0.5$

$0 = a^2 + a \times (0.3) - 1.7 \times 10^{-5} \times 0.5$

Solve quadratic: $a = [H^+] = 2.8 \times 10^{-5}$ M

Calculate: $pH = -\log_{10}(2.8 \times 10^{-5}) = 4.55$

## HOW TO USE THE HENDERSON-HASSELLBACH APPROXIMATION FOR BUFFER PH

Assume that "a" in the previous problem is << $[HAc]_{init}$ and $[Ac-]_{init}$

**Henderson Hasselbach:** $pH = pK_a + \log_{10}\left\{\frac{[A^-]}{[HA]}\right\}$

✎ **Sample:** Examine previous buffer problem:

Given: $[A^-] = [Ac^-] = 0.3$ M; $[HA] = [HAc] = 0.5$ M
$pK_a = pK_a(HAc) = 4.77$

Calculate: $pH = 4.77 + \log_{10}(0.3/0.5)$
$= 4.77 - 0.22 = \mathbf{4.55}$

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 the [HCl].

Equation: $HCl + NaOH \Rightarrow NaCl + H_2O$

This gives 1:1 molar ratio of HCl: NaOH.

At the **equivalence point**: The moles balance, or more conveniently: Mmoles HCl = mmoles NaOH.

**M(HCl)** x vol-acid (mL) = vol-base (mL) x M (NaOH)

**M(HCl)** = vol-base (mL) x M (NaOH)/vol-acid (mL)

Calculate: **M(HCl)** = 25.00 mL x 1.00 M/50.00 mL
= **0.50 M HCl**

⚠ **Pitfall:** Watch the units on volume and molarity work with "L & mole" or "mL & mmole."

# EXAMINATION OF CHEMICAL EQUILIBRIUM

- For a reaction that has not gone to completion: $a A + b B <=> c C + d D$.
- At **equilibrium**, the process is described by the **equilibrium constant, $K_c$**. $K_c = \frac{[C]_{eq}^c [D]_{eq}^d}{[A]_{eq}^a [B]_{eq}^b}$

For all other conditions, the process is described by the **reaction quotient, $Q_c$**: $Q_c = \frac{[C]^c [D]^d}{[A]^a [B]^b}$

**if $Q_c = K_c$, the reaction is at equilibrium**
**if $Q_c > K_c$, the reaction will go to the left**
**if $Q_c < K_c$, the reaction will go to the right**

Gas-phase reactions may be described with $\mathbf{K_p}$, based on reagent partial pressures. These calculations follow the same strategy as $K_c$.

# EXAMINATION OF CHEMICAL EQUILIBRIUM *cont.*

## HOW TO DETERMINE IF THE REACTION IS AT EQUILIBRIUM

**Compare $Q_c$ with $K_c$**

✎ **Sample:** For the reaction: A <=> C, $K_c = 0.60$; the observed [A] = 0.1 and [C] = 0.20.

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

1. $Q_c = [C]/[A] = 0.20/0.10 = 2.0$; $K_c = 0.60$.
2. $Q_c > K_c$; process 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:

$K_c = 0.64$; $[CO]_{init} = [H_2O]_{init} = 0.5$ M:

| | CO(g) + | $H_2O(g)$ <=> | $CO_2$ (g) + | $H_2$ (g) |
|---|---|---|---|---|
| **Init** | $[CO]_{init}$ | $[H_2O]_{init}$ | 0 | 0 |
| **Equil** | $[CO]_{init}$-a | $[H_2O]_{init}$-a | a | a |

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

Identify equilibrium expression:

$K_c = [CO_2]_{eq}[H_2]_{eq}/[CO]_{eq}[H_2O]_{eq}$

Substitute "equil" values:

$K_c = a^2/\{([CO]_{init} - a) \times ([H_2O]_{init} - a)\}$

$0.64 = a^2/\{(0.50 - a)(0.50 - a)\}$

Take square root of each side:

$0.8 = a/(0.5-a)$ or $-0.8 = a/(0.5-a)$

$a = 0.222$ or $a = -1.2$

Use the first option, since "a" must be positive.

$[CO_2]_{eq} = [H_2]_{eq} = 0.222$ M

$[CO]_{eq} = [H_2O]_{eq} = 0.50 - 0.222 = 0.278$ M

Check your work: $K_c = (0.222^2)/(0.278^2) = 0.64$

⚠ **Pitfall:** Watch out for round-off error; take the root that gives positive concentrations.

## HOW TO DETERMINE THE SOLUBILITY LIMIT FROM $K_{SP}$ (GIVEN IN MOLES/L OR G/L)

✎ **Sample:** Determine the solubility limit for silver chloride, AgCl, given $K_{sp} = 1.77 \times 10^{-10}$.

Given: $AgCl(s) <=> Ag^+(aq) + Cl^-(aq)$;
$K_{sp} = [Ag^+][Cl^-] = 1.77 \times 10^{-10}$

Given: AgCl molar mass = 143.32 g/mole

At equilibrium, $[Ag^+]_{eq} = [Cl^-]_{eq} = \sqrt{(K_{sp})}$

Calculate: $[Ag^+]_{eq} = \sqrt{(1.77 \times 10^{-10})}$
$= 1.33 \times 10^{-5}$ M AgCl

This is also $[AgCl]_{eq}$, the **molar solubility limit** for AgCl.

Calculate: The AgCl **g/L solubility limit**
$= [AgCl]_{eq}$ x molar mass of AgCl
$= 1.33 \times 10^{-5}$ moles/L AgCl x 143.32 g/mole
$= \mathbf{1.9 \times 10^{-3}}$ **g/L**

# KINETICS & MECHANISMS

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 REACTION RATE

For "A=>B," the **reaction rate** is the rate of appearance of product, $\Delta[B]/\Delta time$; or, rate of loss of reactant: $-\Delta[A]/\Delta time$.

✎ **Sample:** How would you characterize the rate of: $CaCO_3(s) \Rightarrow CaO(s) + CO_2(g)$?

Answer: Focus on rate of $CO_2$ production; Rate = $\Delta[CO_2]/\Delta time$.

## HOW TO DETERMINE THE RATE LAW

The **rate law** gives the **order** of the reaction based on the steps in the overall reaction "A + B => 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 $[A]^0$, for a zero-order reaction.

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

# KINETICS *cont.*

Two common rate-law methods: "**Initial rates**" and "**integrated rate equations**." Consider the reaction "A=>B," with a rate law of the form: Rate = k $[A]^x$. The goal of kinetic study: Determine "x," the order of the reaction.

**1. Initial Rate Strategy:**

Step 1: For $[A]_1$, measure the time required to produce $\Delta[B]$ of product.

Calculate: $Rate_1 = \Delta[B]/time$

Step 2: Measure the new reaction rate, $rate_2$, for a different concentration, $[A]_2$.

The interplay of rate, [A] and x, are governed by the equation: $\frac{Rate_1}{Rate_2} = \left\{\frac{[A]_1}{[A]_2}\right\}^x$

✎ **Sample:** Determine "x" if doubling [A] also doubles the rate:

1. $Rate_1/Rate_2 = 2$
2. $[A]_1/[A]_2 = 2$
3. $2 = 2^x$, x = 1, this is a 1st order process

✎ **Sample:** Determine "x" if doubling [A] increases the rate by 4-fold:

1. $Rate_1/Rate_2 = 4$
2. $[A]_1/[A]_2 = 2$
3. $4 = 2^x$, x = 2, this is a 2nd order process

**2. Integrated Rate Equation Strategy**

Analyze "[A] vs. time" data for the reaction.

The reaction is 1st order if the "ln [A] vs. t" graph is linear.

The reaction is 2nd order if "1/[A] vs t" graph is linear.

In each case, k is the slope of the line.

## HOW TO DETERMINE THE ACTIVATION ENERGY, $E_a$

$$\ln(k_1/k_2) = -E_a/R\,(1/T_1 - 1/T_2)$$
$$= E_a/R\,(T_1 - T_2)/(T_1 \times T_2)$$

Applications:

a. Predict $k_1$ at $T_1$, given $k_2$ at a $T_2$ and $E_a$.
b. Determine $E_a$ from $k_1$, $k_2$, $T_1$, $T_2$; only have to worry about $k_1/k_2$.

**Sample:** The rate constant doubles when the temperature changes from 25.0°C to 50.0°C. What is $E_a$?

Given: $k_1/k_2 = 2$

Calculate: $T_1$ = 50.0°C + 273.15 = 323.2 K

Calculate: $T_2$ = 25.0°C + 273.15 = 298.2 K

Calculate: $\Delta T = T_1 - T_2 = 25.0$ K

Calculate: $E_a = R \ln(k_1/k_2)\, T_1 \times T_2/\Delta T$
= 8.314 J/mole K x ln (2) x 323.2 K
x 298.2 K/25.0 K
= 22,200 J/mole = 22.2 kJ/mole

⚠ **Pitfall:** T must be in Kelvin; if you use the equation with "$1/T_1 - 1/T_2$," beware of round-off error in calculating inverse T.

## KINETICS & EQUILIBRIUM

An equilibrium is characterized by competing forward and reverse reactions. The forward and reverse **rate constants** ($k_f$ and $k_r$) are related to the equilibrium constant, $K_{eq}$. At equilibrium: The forward and reverse reaction rates are **equal**. $\mathbf{k_{eq} = k_f / k_r}$

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**CREDITS**
**Author:** Mark Jackson, PhD.
**Layout:** André Brisson

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**Note:** Due to the condensed nature of this guide, use as a quick reference guide, not as a replacement for assigned course work.

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