

Queen's **CHEM 112A**

Winter 2025, Chapter 1 Notes



Table of Contents

Chapter 1. Introduction

1.1. Scientific Method

1.1.1. The Scientific Method

1.1.2. Example

1.1.3. Example

1.1.4. Practice

1.1.5. Practice

1.2. Classifying Matter

1.2.1. Classifying Matter

1.3. Physical Properties

1.3.1. Physical Properties

1.4. Extensive vs Intensive Properties

1.4.1. Extensive vs Intensive Properties

1.5. Chemical vs Physical Changes

1.5.1. Chemical vs Physical Changes

1.5.2. Practice

1.6. SI Units

1.6.1. SI Units

1.7. Significant Digits

1.7.1. Significant Digits

1.7.2. Example

1.8. Dimensional Analysis

1.8.1. Dimensional Analysis

1.9. Mathematical Concepts

1.9.1. Scientific notation

1.9.2. Scientific Notation Practice

1.10. Atomic Structure

1.10.1. The Atom and its Subatomic Particles

1.10.2. Example

1.10.3. Practice

1.11. Atoms, Molecules, and the Mole!

1.11.1. Moles

1.11.2. Example

1.11.3. Practice

1.11.4. Practice

1.12. Introduction to Chemical Equations and Balancing

1.12.1. Balancing Reactions

1.12.2. Reaction Stoichiometry

1.12.3. Example

1.12.4. Polyatomic Ions

1.12.5. Example

1.12.6. Practice

1.13. Stoichiometry

1.13.1. Intro to Stoichiometry

1.13.2. Stoichiometry: Putting it All Together

1.13.3. Example

1.13.4. Example

1.13.5. Practice

1.13.6. Practice

1.14. Limiting Reagents

1.14.1. Introduction to Limiting Reagents

1.14.2. Example

1.14.3. Example

1.14.4. Example

1.14.5. Practice

1.15. Percent Yield

1.15.1. Percent Yield

1.15.2. Example

1.15.3. Practice

1.15.4. Practice

1.16. Oxidation States

1.16.1. Oxidation States

1.16.2. Oxidation States - Additional Information

1.16.3. Example

1.16.4. Practice

1.16.5. Practice

1.17. Reduction-Oxidation (Redox) Reactions

1.17.1. Redox Reactions Theory

1.17.2. Practice

1.17.3. Practice

1.17.4. Practice

1.18. Naming Compounds

1.18.1. Naming Compounds

1.18.2. Example

1.18.3. Example

1.18.4. Example

1.18.5. Practice

1.19. Introductory Nomenclature

1.19.1. Types of Formula and Compounds

1.19.2. Oxidation States

1.19.3. Example: Oxidation States in the Hydroxide Ion

1.19.4. Practice: Oxidation State of Sulphur in Sulphate and Sulphite

1.19.5. Practice: Oxidation State of Carbon in Methane

1.20. Organic Nomenclature

1.20.1. Functional Groups

1.20.2. Functional Group Parent Names

1.20.3. Functional Group Identification Practice

1.20.4. Naming Simple Hydrocarbons

1.20.5. Hydrocarbon Example

1.20.6. Steps to Naming Complex Organic Molecules

1.20.7. Naming Organic Molecules with Odd Functional Groups

1.20.8. Nomenclature Practice

1.21. Conformations and Stereochemistry

1.21.1. Conformations and Stereochemistry Introduction

1.21.2. E vs Z

1.21.3. Concept Clarifier

1.21.4. Optical Isomers, R vs S

1.21.5. Asymmetric Centers Example

1.21.6. Unrelated vs Diastereomers vs Enantiomers vs Identical

1.21.7. Newman Projections

1.21.8. Rotomers of 2-methylbutane

1.21.9. Cyclohexane Rings

1.21.10. Isomer Summary

1.Q. Exam Questions & Practise

1. Introduction

1.1 Scientific Method

1.1.1

The Scientific Method

This is the process scientists use to understand everything in the universe. Using this system we can guard against false conclusions.

Scientific Approach

Observations lead to questions

Answer questions using:

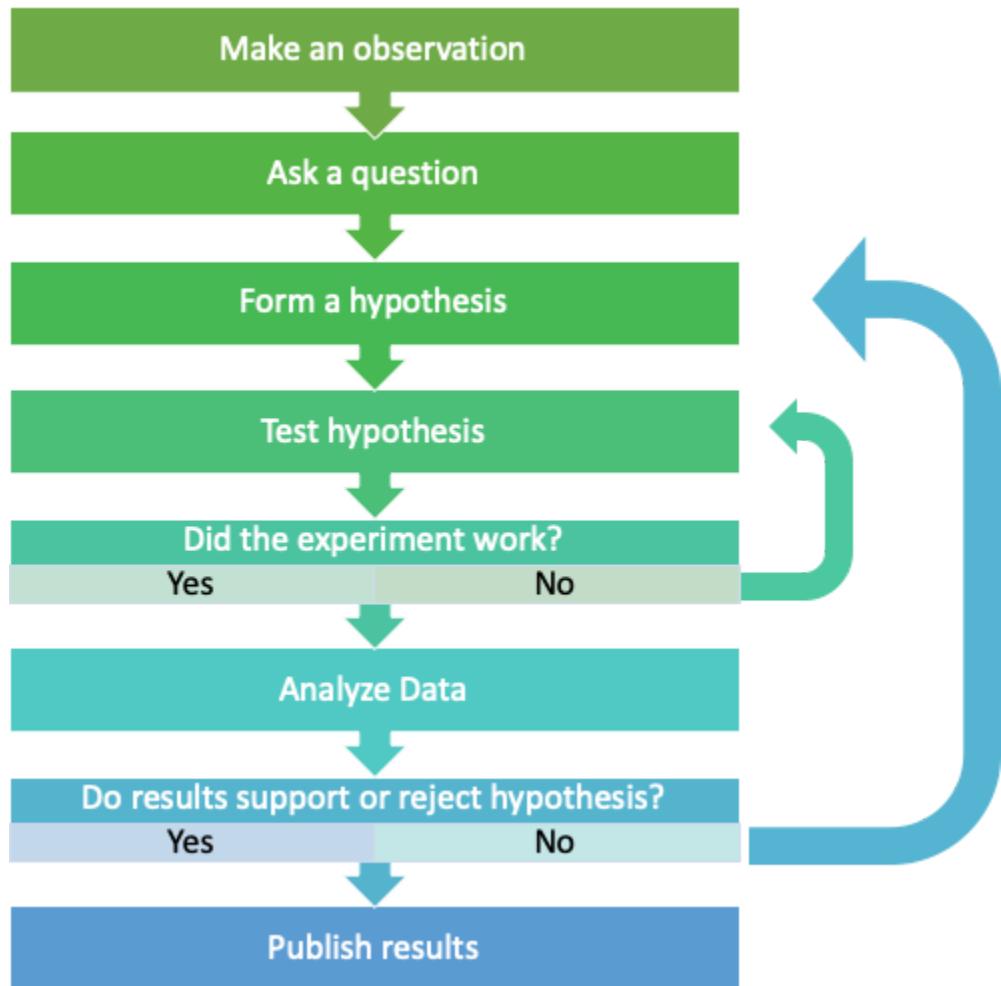
- **Observation:** No manipulation
- **Experimentation:** Controlled studies

Studies designed to test **hypotheses**

- Hypotheses must be **falsifiable**: we can test them and accept or reject the hypothesis
 - Data can support hypotheses, but never **prove** them

Scientific Method

The process scientists use to understand the world



Example: Scientific Method

Applying the Scientific Method

When walking in the woods, you notice that two types of flowers (a red flower and a blue flower) are always found growing next to each other.

Using the Scientific Method, develop a hypothesis about the observation, then design an experiment to test that hypothesis.

1.) Observation

2.) Question

3.) Hypothesis

4.) Test the hypothesis

Example: Scientific Method

After walking through the garden you notice that the bees are all hovering around one type of purple flower.

This represents a(n) _____.

1. Hypothesis
2. Analysis
3. Observation
4. Experiment

1.1.4

Practice: Hypotheses

A hypothesis needs to be _____.

General

Falsifiable

Predictive

Novel

1.1.5

Practice: Scientific Method

After a researcher comes up with an interesting scientific question to answer, what is the first step in the scientific method the researcher must take?

gather data

develop general theory

formulate hypotheses

make observations

1.2

Classifying Matter

1.2.1

Classifying Matter

Matter refers to either a solid, liquid, or gas.

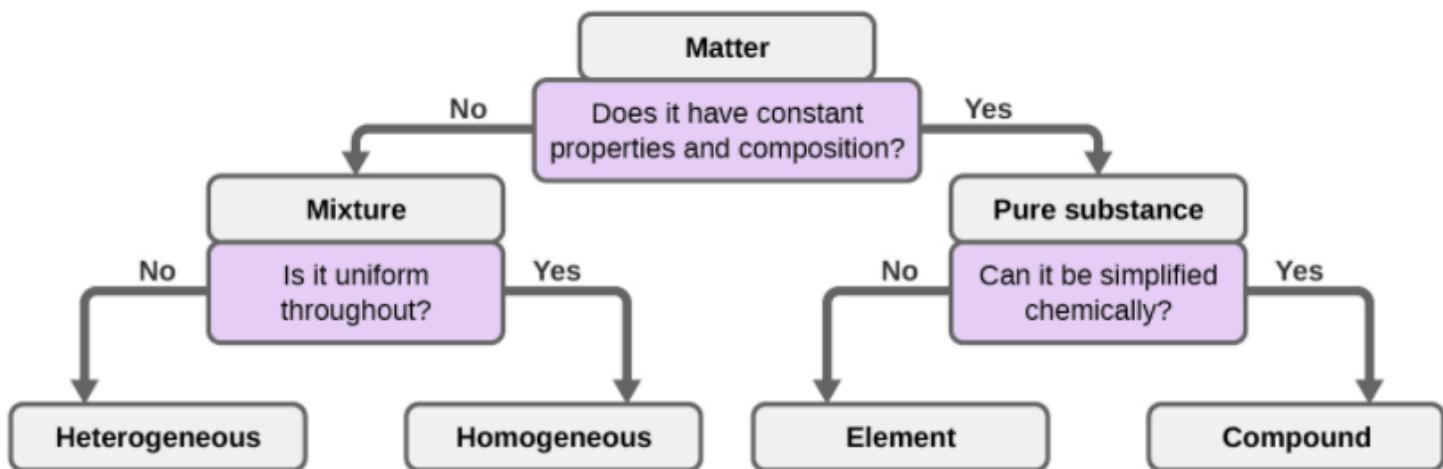


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We can either have **heterogeneous matter** or **homogeneous matter**:

- **Heterogeneous matter:** non-uniform composition
- **Homogeneous matter:** uniform in composition
 - Heterogeneous matter can be separated into homogeneous matter
 - Sometimes you can only tell if something is homogeneous or heterogeneous matter by looking at it under the microscope.
Example: if we just look at blood with our eyes, it looks like it is made of one thing, but if we look at it under a microscope, we can see that there are many components-white blood cells, red blood cells, etc so blood is actually

Example:

Is this a heterogeneous mixture or a homogeneous mixture?



Photo by Talk / CC BY

Homogeneous matter can be either a **solution/mixture** or **pure substance**:

- **Solution:** is a homogeneous mixture because it looks like it is uniform in composition, but it is really made of many different things

Examples: tea! (has water and tea mixed together)

- **Pure substance:** cannot be further purified

- Since a solution is made of more than one component, you can separate it into pure substances (these methods are not perfect!)

To separate a solution to try and get something in it's pure form you could:

- Use **filtration**-separate based on size (bigger components are held back in a net, and smaller components able to filter through)
- Use **distillation**-separates based on volatility (or boiling point)
 - liquids that are most volatile (or have the lowest bps) are separated out first
- Use **chromatography**-a mixture of components can be separated as the mobile phase moves up the plate.

Filtration:

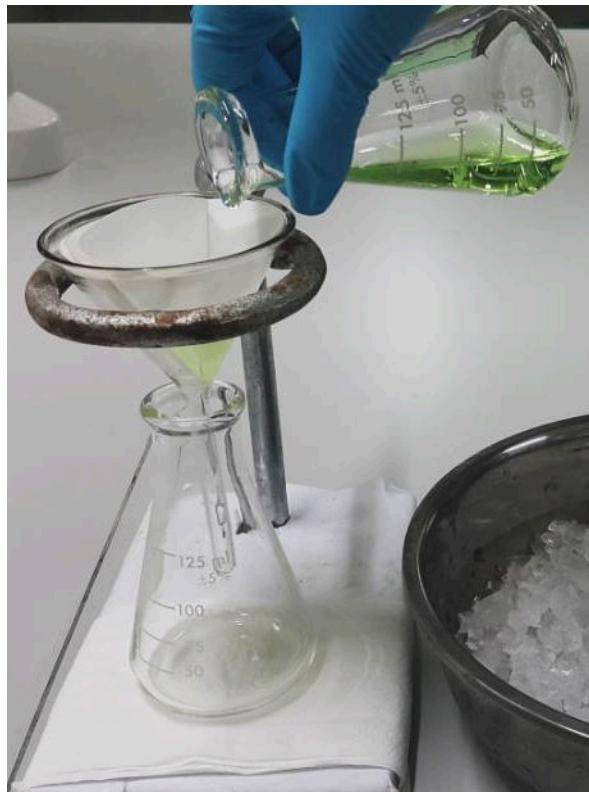


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Distillation:

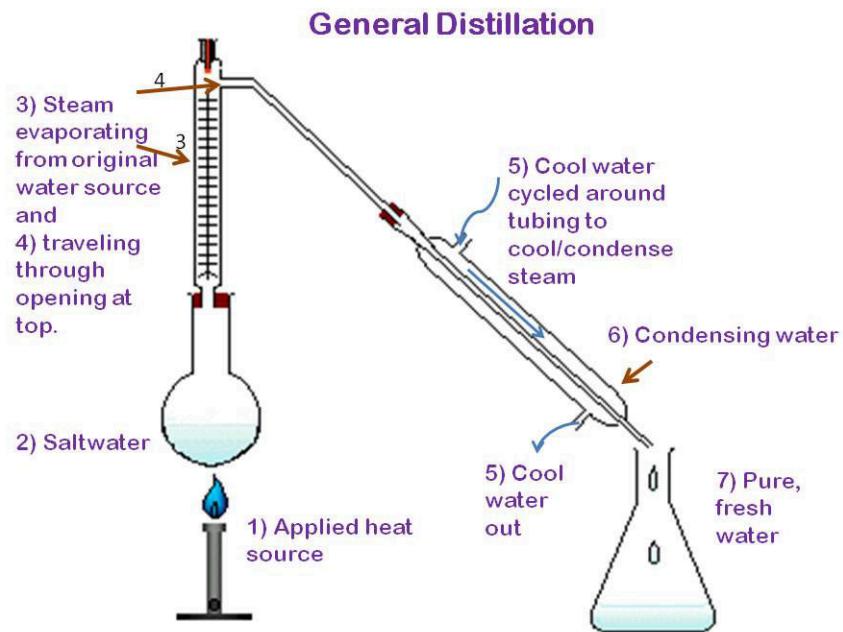


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Chromatography:

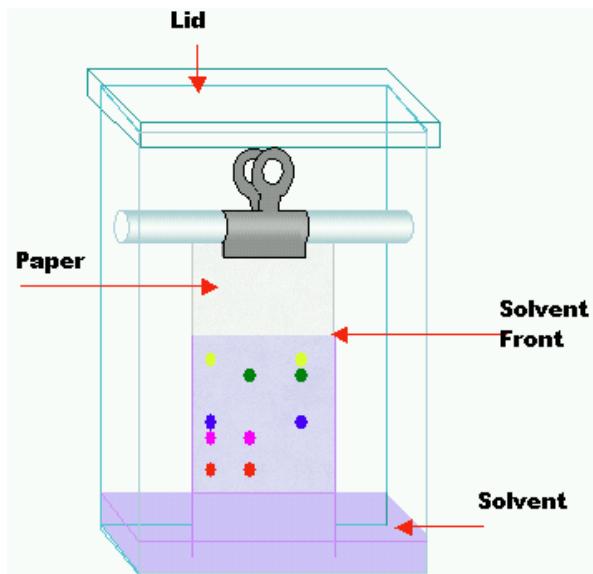


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Finally, **pure substances** can be either **elements** or **compounds**

- **Elements:** can't be subdivided into anything else
- **Compounds:** are made up of elements
 - We can react elements together to form compounds (ex. $2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{g})$)
 - We can separate compounds to form elements (one way to do this is electrolysis)

1.3 Physical Properties

1.3.1

Physical Properties

We use physical properties to help us distinguish different substances. A **physical property** is any property of matter that can be measured.

Colour

- is the substance coloured?
- if it is how intense? What colour?

State of Matter

- Solid, liquid or gas?
- if solid, what shape is it?

Melting Point

- what temperature does a solid melt at?

Boiling Point

- what temperature does a liquid boil at?

Density

- What is the density of the substance?
- $\text{density} = \frac{\text{mass}}{\text{volume}}$
- could be g/mL or g mL⁻¹ or g/cm³ or g cm⁻³
- 1mL=1cm³

Solubility

- what mass of a substance can dissolve in a given volume of a certain solvent

Electric conductivity

- is this substance a conductor of electricity or an insulator?

Malleability

- How easily can the solid be deformed?

Ductility

- How easily can a solid be drawn into a wire?

Viscosity

- How easily does a liquid flow? (think: ketchup vs water!)

1.4

Extensive vs Intensive Properties

1.4.1

Extensive vs. Intensive Properties

Extensive properties: depend on the **EXTENT (or amount)** of a substance

Examples: mass, volume, amount of heat released in a combustion reaction

Intensive properties: does not depend on the amount of substance

Examples: melting point, boiling point, density

No matter how much water you are boiling in a pot, water will always boil at 100°C and melt at 0°C !

When we take a ratio of 2 extensive properties what type of property do we get? (extensive or intensive)

Example: mass/volume=density

1.5

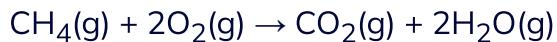
Chemical vs Physical Changes

1.5.1

Chemical vs Physical Changes

A **chemical change** is when bonds are broken and formed between different atoms

Example: Burning a compound in a chemical reaction is an example of a chemical change. The compound is changed as a result of the burning and can't be changed back (we **get a new compound!**)



A **physical change** does not involve the breaking and forming of bonds. Instead, these involve a **change of state**



Example: When ice melts, we have liquid water. Ice is $\text{H}_2\text{O}(s)$ while water is $\text{H}_2\text{O}(l)$. The compound is still the same and could be frozen again to become ice again!



Practice: Chemical vs Physical Changes

Are the following changes physical or chemical changes?

A Change to a Compound	Chemical or Physical Change (Enter answer as C or P)
Seeing bubbles during a reaction	_____
Feeling heat on the outside of a beaker during a reaction	_____
Boiling the compound	_____
Seeing a precipitate form in solution	_____
Seeing light given off of the compound during the reaction	_____
Melting the compound	_____
Seeing a new compound form during the reaction	_____

1.6 SI Units

1.6.1

SI Units

The following units are important for chemistry:

Length- meter (m)
Time- second (s)
Mass- kilogram (kg)
Temperature- kelvin (K)
Amount of a substance- mole (mol)

Sometimes we will see these prefixes being used when units are smaller/larger than the above base SI units:

Common Unit Prefixes

Prefix	Symbol	Factor	Example
femto	f	10^{-15}	1 femtosecond (fs) = 1×10^{-15} s (0.000000000000001 s)
pico	p	10^{-12}	1 picometer (pm) = 1×10^{-12} m (0.000000000001 m)
nano	n	10^{-9}	4 nanograms (ng) = 4×10^{-9} g (0.00000004 g)
micro	μ	10^{-6}	1 microliter (μ L) = 1×10^{-6} L (0.000001 L)
milli	m	10^{-3}	2 millimoles (mmol) = 2×10^{-3} mol (0.002 mol)
centi	c	10^{-2}	7 centimeters (cm) = 7×10^{-2} m (0.07 m)
deci	d	10^{-1}	1 deciliter (dL) = 1×10^{-1} L (0.1 L)
kilo	k	10^3	1 kilometer (km) = 1×10^3 m (1000 m)
mega	M	10^6	3 megahertz (MHz) = 3×10^6 Hz (3,000,000 Hz)
giga	G	10^9	8 gigayears (Gyr) = 8×10^9 yr (8,000,000,000 yr)
tera	T	10^{12}	5 terawatts (TW) = 5×10^{12} W (5,000,000,000,000 W)

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Other Important Units for Chemistry

- Relationship between L and mL (1 L=1000 mL)
- The Angstrom (\AA) is $1 \times 10^{-10}\text{m}$ (low yield)
 - Used in chemistry because it is a very tiny value, perfect for using when measuring the size of an atom or molecules!

1.7 Significant Digits

1.7.1

Significant Digits

Significant digits (aka significant figures) indicate the precision of a measurement and determine how precisely a calculated number can be represented.

To count the significant figures in a value, follow these steps while reading from left to right through the number:

- 1) Start counting at the first non-zero digit

Example:

0.0095 → _____

- 2) If a digit is not zero, it is significant

Example:

456 → _____

- 3) If a digit is zero and there are nonzero digits or a decimal ahead, it is significant

Examples:

1290. → _____

12900 → _____

- 4) If a digit is zero and it occurs after a decimal point, it is significant

Example:

52.00 → _____

Adding and Subtracting

When adding or subtracting measurements, the **number with the least digits beyond the decimal point sets the limit for the answer**. Any extra digits must be rounded off.

Examples:

$$4.3568\text{g} - 0.14\text{g}$$

$$100\text{mL} + 150.47\text{mL}$$

Multiplying and Dividing

When multiplying or dividing measurements, the **number with the least significant figures sets the limit for the answer.**

Any extra digits must be rounded off.

Examples:

$$49.63\text{m} \times 36\text{m}$$

$$57.6\text{kPa}/101.325\text{kPa}$$

$$0.0076 \times 1.2455$$

Accuracy and Precision

Accuracy: how closely a measurement aligns with a correct value

Precision: how closely a measurement matches the same measurement when repeated

Example: Significant Digits

How many significant digits do the following numbers have?

$$0.00045 \rightarrow \underline{\quad}$$

$$234000 \rightarrow \underline{\quad}$$

$$234000.0 \rightarrow \underline{\quad}$$

1.8 Dimensional Analysis

1.8.1

Dimensional Analysis

This is helpful when converting units or figuring out a way to calculate one quantity without a formula.

Unit Conversion Examples

Convert 4.56 km/h into m/s.

Convert 1.63 Ms to μs .

Calculate the speed of an object which moves 12m in 8s in m/s.

1.9

Mathematical Concepts

1.9.1

Scientific Notation

- Instead of writing very large or very small number we can express these numbers as a number between -10 and positive 10 (exclusively) multiplied by 10^n

Example:

$$62\,000\,000\,000 = 6.2 \times 10^{10}$$

1.9.2

Write the following in scientific notation:

$$584 =$$

$$4,529,000 =$$

$$78,000,000 =$$

$$0.00000128 =$$

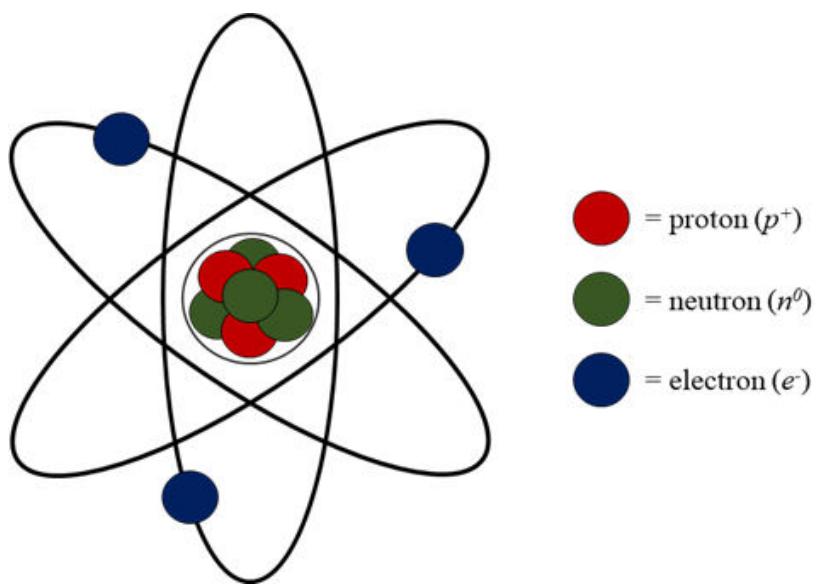
1.10 Atomic Structure

1.10.1

The Atom and its Subatomic Particles

Atoms are the building blocks of chemistry (and life!). They make up everything from the screen of your computer, to components in your eyes! They are all around us. Since atoms are such a key concept in chemistry, let's take a closer look at their structure.

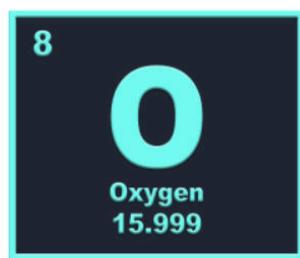
Atomic Structure



Subatomic Particles

Particle	Mass (g)	Mass (amu or g·mol ⁻¹)	Relative Charge
Proton	1.673×10^{-24}	1.007	+1
Neutron	1.675×10^{-24}	1.009	0
Electron	9.109×10^{-28}	5.485×10^{-4}	-1

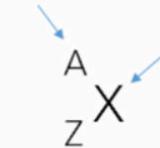
Chemical Symbols and Notation



atomic mass = protons + neutrons

chemical symbol for the element

atomic number= number of protons



Example: Nuclear Notation

Ex1) $^{12}_6C$

of protons: _____

of neutrons: _____

of electrons: _____

WIZE CONCEPT

Atomic Mass = # of protons + # of neutrons

of neutrons = Atomic mass - # of protons

Ex2) $^{19}_9F^-$

of protons: _____

of neutrons: _____

of electrons: _____

WIZE TIP

When electrons are added to an element we call it an **anion**, and it would have a **negative charge**.

When electrons are removed from an element we call it a **cation**, and it would have a **positive charge**

1.10.3

Practice: Nuclear Notation

How many protons, neutrons and electrons are there in $^{75}As^{3-}$?

Number of protons

Number of neutrons

Number of electrons

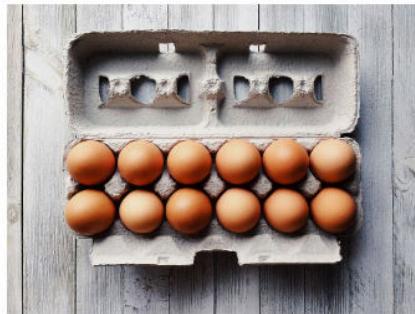
1.11

Atoms, Molecules, and the Mole!

1.11.1

Moles

When someone says they want a dozen donuts, roses, or eggs we know they mean they want 12. A **mole** in chemistry also tells us the amount of something.



- Just like how a dozen of something = 12, 1 mole of something = 6.02×10^{23} molecules
- 6.02×10^{23} is referred to as **Avagadro's number (N_A)**

i WIZE TIP

You should memorize Avagadro's number since it is not always provided on exams! We'll soon see that you need to know it to solve problems :)

$$N_A = 6.02 \times 10^{23} \text{ molecules/mole}$$

We use the unit "**moles**" to help make very small amounts more measurable. A mole is just like any other unit!

There are 2 Equations Related to Moles:

$$n = \frac{m}{M}$$

$$n = \frac{N}{N_A}$$

n =# of moles

m =mass (g)

M =molar mass (g/mol)

N =# of molecules or atoms

N_A =Avagadro's number=6.02x10²³ molecules

Example #1:

If we are told that a sample of CO₂(s) weighs 11g, how many moles are present?

Example #2

We have 2 moles of CO₂ present in our sample, how many molecules are there?

Example #3

How many oxygen atoms there in 1 mole of CO₂?

1) Find Number of Molecules In the Sample

2) Find the Number of O atoms in the Sample

In each molecule there are _____ O atoms.

Therefore to find the number of O atoms:

of molecules in sample x _____ O atoms/molecule =# of O atoms

of O atoms= _____

Example: Calculate the Number of Molecules of Ethyl Mercaptan

The volatile liquid ethyl mercaptan, C_2H_6S , is one of the most odoriferous substances known. It is added to natural gas to make gas leaks detectable. ($d = 0.84 \text{ g/mL}$; $MW = 62.1 \text{ g/mol}$)

1. How many C_2H_6S molecules are contained in a $3.0 \mu L$ sample?

2. In the same 3.0 μL sample, how many C and H atoms are there?

1.11.3

Practice: Converting Mass to Number of Atoms

Calculate the number of nitrogen atoms in 2.25 g of bismuth(III) nitrate.

a) 1.03×10^{22} atoms

b) 1.03×10^{21} atoms

c) 3.43×10^{21} atoms

d) 3.43×10^{22} atoms

1.11.4

Practice: Finding the Number of Moles of Iron

Calculate the number of moles of iron atoms in 14.1 g of iron oxide, Fe_2O_3

A) 0.177 mol

B) 0.0821 mol

C) 0.0906 mol

D) 0.0451 mol

1.12 Introduction to Chemical Equations and Balancing

1.12.1

Balancing Reactions

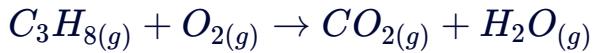
Reactions must be balanced before the stoichiometry can be analyzed.

What makes a reaction balanced?

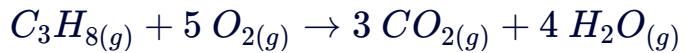
The number of _____ of each type on the _____ must equal the number of atoms of each type on the _____ of the reaction.

Example:

Unbalanced:

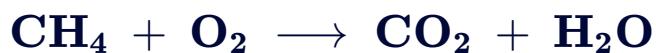


Balanced:



Balancing Chemical Reactions

Unbalanced Reaction



The **subscripts** tell us the ratio of different atoms in one molecule.

Example: One CH₄ molecule has 4 hydrogen atoms and 1 carbon atom

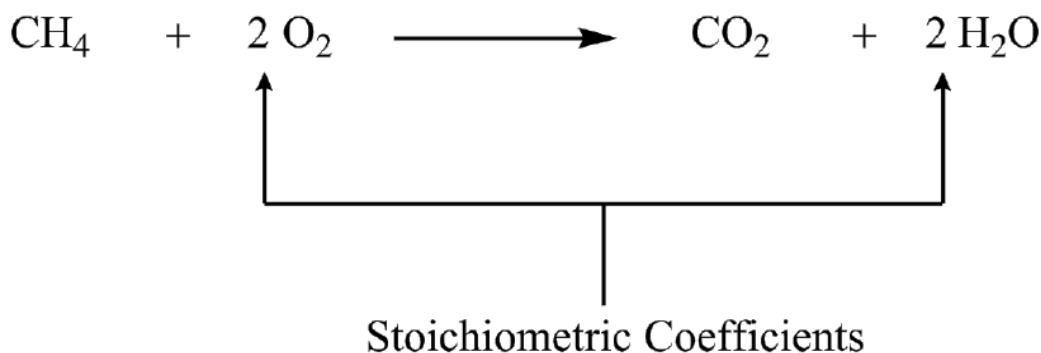
WATCH OUT!

Sometimes you could be given unbalanced equations and you are expected to balance them!
We **need to use the balanced equation for calculations** in order to get the correct answer!

Steps to Balance Chemical Equations

1. Balance **elements that only appear once** on the reactant side and once on the product side (typically elements not including C, N, H, O)
2. **Group polyatomic ions** and balance them as a group (not as separate elements, e.g. balance NO_3 as 1 NO_3 group, not 1 N and 3 O)
3. **Balance all other elements**, starting with the least common elements to the most common elements
4. Make sure all **coefficients are whole numbers** AND are represented in the **simplest integer ratio possible**
5. **Check** to make sure all elements are balanced on each side of the chemical equation

Balanced Reaction



- The **stoichiometric coefficients** of the balanced equation tell us that we need _____ oxygen molecules for each methane (CH_4) molecule and we produce _____ waters for every methane consumed.
- It also tells us that for every 1 mole of methane used we produce _____ mole of CO_2 .

WIZE CONCEPT

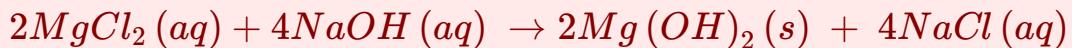
Multiply coefficients by subscripts to see exactly how much of an atom we have on each side.

! WATCH OUT!

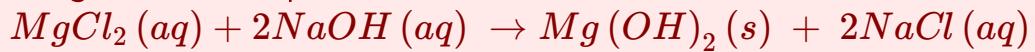
We want the **lowest possible coefficients**.

Example:

If I balanced an equation and got:



The **greatest common factor** that can go into each coefficient is 2 so we need to divide each coefficient by 2 to get the lowest possible numbers!



Example: Balancing a Chemical Reaction

Balance the following equation:



WIZE CONCEPT

The physical state of each chemical compound is often included in chemical equations:

(s) = solid

(l) = liquid

(g) = gas

(aq) = aqueous

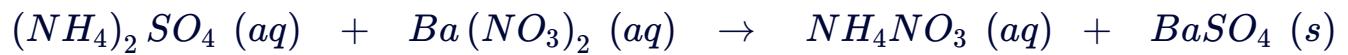
Polyatomic Ions

Note: There is no need to memorize the following table. It is just included here so you have an idea about what a polyatomic ion is!

Polyatomic Ion Cheatsheet			
Ion	Name	Ion	Name
NH_4^+	Ammonium	MnO_4^-	Permanganate
NO_2^-	Nitrite	CrO_4^{2-}	Chromate
NO_3^-	Nitrate	$\text{Cr}_2\text{O}_7^{2-}$	Dichromate
SO_3^{2-}	Sulfite	O_2^{2-}	Peroxide
SO_4^{2-}	Sulfate	O_2^-	Superoxide
HSO_4^-	Hydrogen sulfate *	$\text{C}_2\text{O}_4^{2-}$	Oxalate
HSO_3^-	Hydrogen sulfite	HC_2O_4^-	Hydrogen Oxalate
OH^-	Hydroxide	HCO_2^-	Formate
CN^-	Cyanide	$\text{S}_2\text{O}_3^{2-}$	Thiosulfate
PO_4^{3-}	Phosphate	HS_2O_3^-	Hydrogen Thiosulfate
HPO_4^{2-}	Hydrogen Phosphate	BrO_4^-	Perbromate
H_2PO_4^-	Dihydrogen Phosphate	BrO_3^-	Bromate
CO_3^{2-}	Carbonate	BrO_2^-	Bromite
HCO_3^-	Hydrogen Carbonate **	BrO^-	Hypobromite
ClO^-	Hypochlorite	IO_4^-	Periodate
ClO_2^-	Chlorite	IO_3^-	Iodate
ClO_3^-	Chlorate	IO_2^-	Iodite
ClO_4^-	Perchlorate	IO^-	Hypoiodate
$\text{C}_2\text{H}_3\text{O}_2^-$	Acetate		

1.12.5

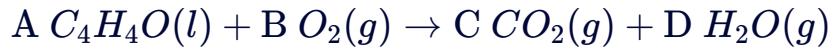
Example: Balance a Chemical Equation with Polyatomic Ions



1.12.6

Practice: Balancing the Combustion of Furan

Choose the answer that balances the reaction shown below:



A = 2; B = 9 ;C = 8; D = 4

A = 1; B = 3 ;C = 5; D = 2

A = 1; B = 1 ;C = 1; D = 1

A = 4; B = 25 ;C = 20; D = 10

1.13 Stoichiometry

1.13.1

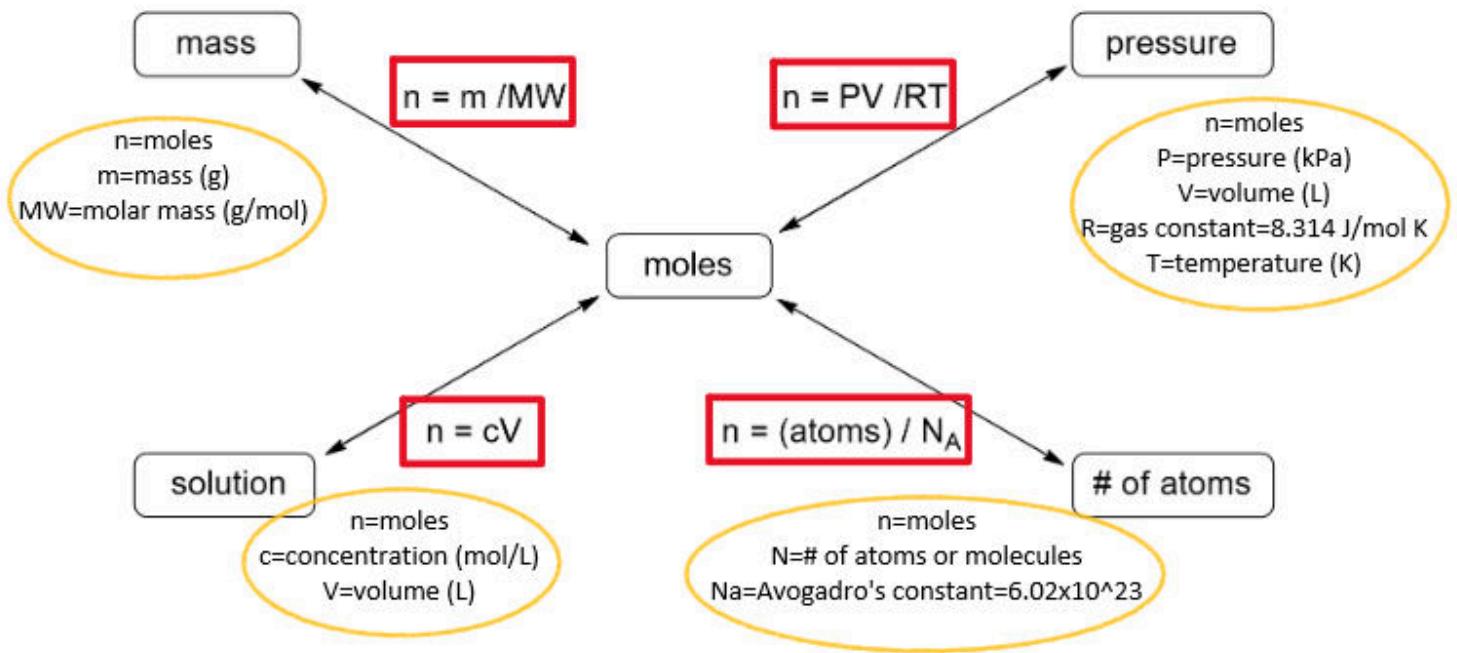
Intro to Stoichiometry

Stoichiometry allows us to predict the quantities of products or reagents across a chemical reaction.

Typically this is done in a few steps:

1. Calculating the number of moles of the reagents
2. Calculating the number of moles of the products using the stoichiometric ratio
3. Calculating the mass or pressure of the products.

Moles are the central unit!



In addition we can convert between mass and volume of a pure substance by looking at it's **density**,

$$\delta = m/V$$

Stoichiometry of a Reaction

We use the **coefficients** of the **balanced reaction** along with the our equations that convert mass, volume, and concentration into moles to predict the quantities of reactants and products in a chemical reaction.

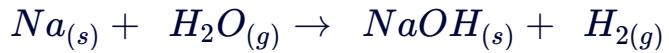
To answer any stoichiometry problem, focus on converting to and from moles!

General Steps to Solving a Stoichiometry Problem:

1. Convert the values given in the problem about a reactant or product to a **number of moles**
2. Use the **stoichiometric coefficients** from the **balanced** reaction to **find the number of moles of the unknown** you are being asked for
3. Convert the number of moles of your unknown to a mass, or whatever quantity you are being asked for

Example

2.6g of sodium metal (Na) reacts with water to form NaOH and H₂ according to the unbalanced reaction below. Once the reaction is complete how many grams of NaOH are formed?



i WIZE TIP

On an exam, your prof will NOT specify if an equation is balanced or unbalanced.

Always double check that the equation is balanced. If it's not, balance the equation before continuing!

The equation must be balanced in order to get the correct answer!

Step 1: Balance the reaction



Step 2: Find the number of moles of sodium

$$n_{\text{Na}} = \frac{m}{MW} = \frac{2.6 \text{ g}}{22.990 \text{ g/mol}} = 0.113 \text{ mol}$$

Step 3: Find the number of moles of NaOH

$$n_{\text{NaOH}} = n_{\text{Na}} \times \frac{\text{coefficient NaOH}}{\text{coefficient Na}} = 0.113 \text{ mol} \times \frac{2}{2} = 0.113 \text{ mol}$$

Step 4: Convert the number of moles of NaOH to a mass

$$n = \frac{m}{M}$$

$$m_{\text{NaOH}} = n \times MW = 0.113 \text{ mol} \times 39.997 \text{ g/mol} = 4.520 \text{ g} = 4.5 \text{ g}$$

1.13.3

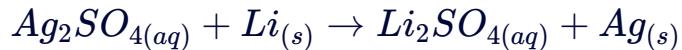
Example: Converting Mass of Reactant to Mass of Product

Calculate the mass of hydrogen gas produced if 0.550 g of iron powder is reacted with an excess amount of sulfuric acid.



Example: Solution Stoichiometry to Determine Mass of Product

Lithium metal was added to a 25mL of a 1.3M solution of Ag_2SO_4 . The unbalanced chemical reaction is shown below.



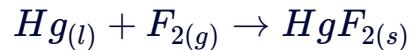
Once the reaction has gone to completion, what mass of silver metal is produced?

- a) 0.0070 g
- b) 7.0 g
- c) 3.5 g
- d) 0.0035 g

1.13.5

Practice: Calculate the Mass of Product

16.0 mL of Hg (mp = -38.8°C, density = 13.56 g/mL) reacts with fluorine gas and the reaction goes to completion as shown below.



Once the reaction has gone to completion, what mass of mercury fluoride, HgF_2 , is produced?

A) 1.48 g

B) 514 g

C) 142 g

D) 258 g

1.13.6

Practice: Stoichiometry Calculations Application

A solution that is 183mM (millimolar) NaCl(aq) is isoosmotic with plasma. This means that cells don't swell or shrink when in this solution. How many grams of sodium chloride are required to make 150mL of isoosmotic NaCl(aq)? The molar mass of NaCl is 58.44g/mol.

0.2g



1.6g



2.2g



4.9g



1.14 Limiting Reagents

1.14.1

Introduction to Limiting Reagents

Anytime **reactant species are in limited supply** and not present in perfectly proportional amounts, a chemical reaction will have a **limiting reagent** which will be totally **consumed before any other reactant**

The quantity of the limiting reagent available directly **determines the maximum number of product molecules** that can be formed!

Let's Consider an Example:

When making smores (yum!!) the "reaction" looks something like:



If I had 10 graham crackers, 6 pieces of chocolate, and 6 marshmallows, what would be the limiting reagent? In other words, what would I run out of first? And how many smores could I make?

- The "chemistry way" to figure this out would be to **take the # of moles of each reactant and divide by its stoichiometric coefficient**:

Graham crackers: $10/2=5$

Pieces of chocolate: $6/1=6$

Marshmallows: $6/1=6$

- Now, **to figure out the limiting reagent, look at which of the above numbers are the smallest!!**
 - 5 is smallest, therefore Graham crackers are the limiting reagent!!

Now how many smores could we make?

We know graham crackers will determine how much product we get since we'll run out of the crackers first.

$$\text{moles of graham cracker} \times \frac{1 \text{ mol smores}}{2 \text{ moles graham cracker}} = \text{moles of smores}$$

 **WIZE CONCEPT**

It is necessary to **determine the limiting reagent** whenever we are **given the amounts of two or more reactants** in a chemical reaction.

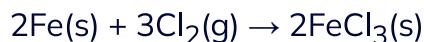
The limiting reagent is **totally consumed in the reaction. Any other reactant is in excess.**

Limiting reagent stops the reaction by **running out first.**

The **quantity of the limiting reagent** available directly **determines the maximum number of products molecules** that can be formed

Example: Determine the Mass of Product in a Limiting Reagent Problem

Iron and chlorine gas react to form iron (III) trichloride. If 110 g of iron and 105 g of chlorine gas are reacted, which species is the limiting reagent? What is the maximum mass of FeCl_3 that can be formed?



 **WIZE TIP**

Steps for Solving Limiting Reagent Problems:

Step 1 – Write & **balance** the equation.

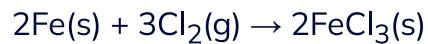
Step 2 – Calculate **moles of each reactant**.

Step 3 – Use the molar ratios of the present reactants (from the balanced equation) to determine the limiting reactant (LR).

- Take the **# of moles of each reactant** from step 2 and **divide by the stoichiometric coefficient** for that reactant
 - **Smallest value** from this calculation tells us the **LR**

Step 4 – From the limiting reactant, use the **molar ratio** (from the balanced equation) to **calculate moles of the desired product**.

Step 5 – Convert moles to the desired units (density, molarity, grams, etc...)



Step 1 – Write & balance the equation.

Is the equation given balanced? _____

Step 2 – Calculate moles of each reactant.

i) Find moles of Fe

ii) Find moles of Cl₂

Step 3 – Use the molar ratios of the present reactants (from the balanced equation) to determine the limiting reactant.

Therefore the limiting reagent is _____ ! (because it had the smallest number)

Step 4 – From the limiting reactant, use the molar ratio (from the balanced equation) to calculate moles of the desired product.

- The maximum mass of FeCl_3 that is formed depends on how much we have (LR).

Step 5 – Convert moles to the desired units (density, molarity, grams, etc...)

Example: What is the Limiting Reagent?

2.0 g of aqueous Barium hydroxide ($\text{Ba}(\text{OH})_2(\text{aq})$, 171.32 g/mol) and 1.5 g of liquid hydrogen bromide ($\text{HBr}(\text{l})$, 80.91g/mol) react together to give aqueous barium bromide ($\text{BaBr}_2(\text{aq})$) and liquid water ($\text{H}_2\text{O}(\text{l})$). Which species would be the limiting reagent of this reaction?

Example: How Many Grams of the Excess Reagent Will Remain?

The reaction between P_4 and Br_2 is very exothermic and produces PBr_5 as the only product. If 7.0 g of P_4 react with 12.0 g of Br_2 how many grams of the excess reagent will remain?

- a) 0.4 g
- b) 4.7 g
- c) 6.1g
- d)11.1 g

1.14.5

Practice: What is the Limiting Reagent

If 12 g of sodium is mixed with 0.64 g of H₂ and 17 g of O₂ which reagent will be limiting in the reaction shown below?



A) Na

B) O₂

C) H₂

D) None, they will all be completely consumed

1.15 Percent Yield

1.15.1

Percent Yield

So far we have been assuming that the reaction proceeds 100% to products. In reality, this is rarely the case!

When we are doing experiments in the lab we often lose some of our product by spilling it or residues of it get left on glassware and spatulas.



So far we have been calculating the **theoretical yield**.

Theoretical Yield - the maximum amount of product produced based on the quantity of the limiting reagent (e.g. the amount of product produced in a calculation).

Actual Yield - the actual amount of product produced in the reaction (e.g. the amount of product obtained in a laboratory experiment).

$$\% \text{ yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

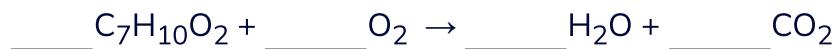
Test Your Understanding

- 1) In a lab, you measure your product and record 5.222g. This is the _____ yield.
- 2) If everything went 100% perfectly according to the reaction we would get the _____ yield
- 3) If I determined the limiting reagent, and then calculated the number of moles of product and the mass of product based on this, I've just calculated the _____ yield

1.15.2

Example: What is the Percent Yield

When 49.00 g of a hydrocarbon fuel with formula $\text{C}_7\text{H}_{10}\text{O}_2$ is reacted with excess oxygen, a total of 21.56 g of water is collected. What was the percent yield of the reaction?



1.15.3

Practice: Calculate Moles Given Percent Yield

If the yield for the following reaction is 45%, how many moles of KClO_3 are needed to produce 1 mol of O_2 ?



A) 0.4 moles

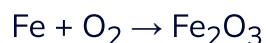
B) 1.1 moles

C) 1.5 moles

D) 4.6 moles

Practice: Limiting Reagent & Percent Yield

Iron oxidizes when exposed to oxygen to form iron oxide according to the following equation:



352g of pure iron is exposed to 12.0 mols of O_2 , and after a period of time 46.7 g of iron oxide (rust) is collected.

Part 1

What is the limiting reagent in this reaction?

A) Fe

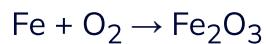
B) O_2

C) Fe_2O_3

D) There is no limiting reagent

Practice: Limiting Reagent & Percent Yield

Iron oxidizes when exposed to oxygen to form iron oxide according to the following equation:



352g of pure iron is exposed to 12.0 mols of O_2 , and after a period of time 46.7 g of iron oxide (rust) is collected.

Part 2

What is the percent yield?

A) 2.2%

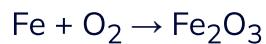
B) 8.8%

C) 9.4%

D) 33.1 %

Practice: Limiting Reagent & Percent Yield

Iron oxidizes when exposed to oxygen to form iron oxide according to the following equation:



352g of pure iron is exposed to 12.0 mols of O_2 , and after a period of time 46.7 g of iron oxide (rust) is collected.

Part 3

How many Fe atoms are present in the rust produced?

A) 0.89×10^{17} atoms

B) 1.77×10^{23} atoms

C) 3.56×10^{23} atoms

D) 4.33×10^{23} atoms

1.16 Oxidation States

1.16.1

Oxidation States

Oxidation state: A way to describe the degree of oxidation of a chemical

 **WIZE TIP**

Tips to Determine Oxidation State:

1. Free elements: oxidation state = 0

Examples: Cl₂(g) has an oxidation state of 0, Na(s) has an oxidation state of 0

2. Monoatomic ions: oxidation state = ionic charge

Examples: Cl⁻(aq) has an oxidation state of -1, Na⁺(aq) has an oxidation state of +1.

3. Hydrogen: oxidation state = +1

a. **Exception: hydrogen in hydrides (e.g., NaH) – oxidation state = -1**

4. Oxygen: oxidation state = -2

a. **Exception: oxygen in peroxides (e.g., H₂O₂) – oxidation state = -1**

5. For neutral molecules, oxidation numbers add up to zero.

For polyatomic ions, oxidation numbers add up to the ion charge.

Examples: Cl₂(g) has an oxidation state of 0, NaCl oxidation numbers add up to 0, SO₄²⁻ oxidation numbers add up to 2-.

Oxidation States - Additional Information

Other Low Yield Tips to Help Determine Oxidation States

- Alkali metals: oxidation state= +1
- Alkaline earth metals: oxidation state= +2
- Nitrogen Group: oxidation state= -3
- Oxygen family: oxidation state= -2
- Halogens: oxidation state= -1

Group →	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
↓ Period																		
1	1 H																2 He	
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Ms	116 Lv	117 Ts	118 Og
Lanthanides	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu			
Actinides	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr			

Note on Transition Metals

Transition metals can have different charges (ex. Pb^{2+} and Pb^{4+})

As a result, transition metals can also have different oxidation states!

Example:

What is the oxidation state of Cu in CuCl ? _____

What is the oxidation state of copper in $\text{Cu}(\text{NO}_3)_2$? _____

When naming compounds involving transition metals, the **oxidation state of the transition metal is written in Roman numerals and put in brackets**:

- copper(I) chloride: CuCl
- copper(II) nitrate: $\text{Cu}(\text{NO}_3)_2$

Example: Oxidation State Practice

What is the oxidation state of:

S in S_2O_3 : _____

O in S_2O_3 : _____

What about Pb in Pb_2O_3 ?

This one is different because this compound is a mixed oxidation state compound, so although Pb should have 2+ or 4+, here, we get an oxidation state of _____ and that is ok because both Pb^{2+} and Pb^{4+} are present in the compound.

1.16.4

What is the oxidation state of Br in BrO_3^- ?

+4

+5

+6

-4

-5

-6

1.16.5

What is the oxidation state for the following: (enter answer as -1 or +2 for example)

a) P in P_2O_5 :

b) Cr in $\text{Na}_2\text{Cr}_2\text{O}_7$:

c) Al in $\text{Al}_2(\text{SO}_4)_3$:

d) Na in Na_2O_2 :

e) O in Na_2O_2 :

f) N in NH_3 :

1.17

Reduction-Oxidation (Redox) Reactions

1.17.1

Redox Reactions

OIL RIG! Oxidation Is Loss of electrons, Reduction Is Gain of electrons
OR

LEO GER! Loss of Electrons is Oxidation, Gain of Electrons is Reduction

OXIDATION (lose e⁻)

REDUCTION (gain e⁻)

Reducing agent reduces others and is itself oxidized.

Oxidation number increases.

Oxidizing agent oxidizes others and is itself reduced.

Oxidation number is reduced.

Keep in mind that in organic chemistry the definitions of oxidation and reduction are different:

- For **reduction**, we would look for **more bonds to H** and **less bonds to O**
- For **oxidation**, we would look for **less bonds to H** and **more bonds to O!**

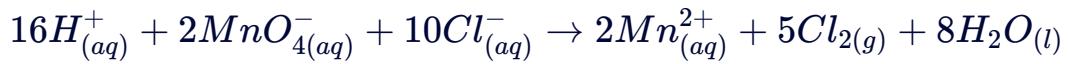
How can you recognize if a redox reaction is occurring?

1. Can check oxidation #s of each element to see if they change from reactants to products (most important for now!)
2. Familiarize yourself with common oxidizing and reducing agents (you'll learn more about this in orgo!)
 - **Oxidizing agents:** O₂, halogens, HNO₃, Cr₂O₇²⁻, MnO₄⁻
 - **Reducing agents:** H₂, metals, C

1.17.2

Practice: Oxidation vs Reduction

Consider the following balanced redox equation:



Which species is being oxidized?

H⁺

MnO₄⁻

Cl⁻

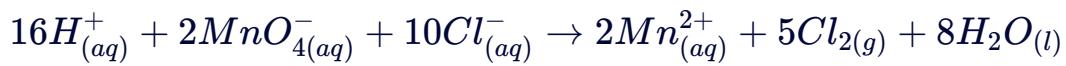
Mn²⁺

Cl₂

1.17.3

Practice: Oxidizing vs Reducing Agent

Consider the following balanced redox equation:



Which species is the reducing agent?

H⁺

MnO₄⁻

Cl⁻

Mn²⁺

Cl₂

1.17.4

Practice: Oxidizing vs Reducing Agents

What is the reducing agent in the following chemical reaction?



Au^+

NO

NO_3^-

Au

1.18 Naming Compounds

1.18.1

Naming Compounds

Naming Ionic Compounds

Ionic compounds are written as a cation (+) followed by an anion (-)

Example: NaCl is made up of Na^+ and Cl^-

i WIZE TIP

Name is written in this format:

[cation's name] [space] [anion's name with "-ide" ending]

Example:

NaCl is sodium chloride

! WATCH OUT!

If the metal (cation) is a **transition metal**, it could have more than one possible oxidation state or "charge".

Indicate the charge in the name using this format:

[transition metal name] (oxidation state in roman numerals) [anion's name with "-ide" ending]

Example:

Fe_2O_3 is iron (III) oxide

Examples:

a) KCl

Ionic or covalent? _____

Name: _____

b) PbO

Ionic or Covalent? _____

Name: _____

Naming Ionic Compounds With Polyatomic Ions

Polyatomic Ion Cheatsheet			
Ion	Name	Ion	Name
NH_4^+	Ammonium	MnO_4^-	Permanganate
NO_2^-	Nitrite	CrO_4^{2-}	Chromate
NO_3^-	Nitrate	$\text{Cr}_2\text{O}_7^{2-}$	Dichromate
SO_3^{2-}	Sulfite	O_2^{2-}	Peroxide
SO_4^{2-}	Sulfate	O_2^-	Superoxide
HSO_4^-	Hydrogen sulfate*	$\text{C}_2\text{O}_4^{2-}$	Oxalate
HSO_3^-	Hydrogen sulfite	HC_2O_4^-	Hydrogen Oxalate
OH^-	Hydroxide	HCO_2^-	Formate
CN^-	Cyanide	$\text{S}_2\text{O}_3^{2-}$	Thiosulfate
PO_4^{3-}	Phosphate	HS_2O_3^-	Hydrogen Thiosulfate
HPO_4^{2-}	Hydrogen Phosphate	BrO_4^-	Perbromate
H_2PO_4^+	Dihydrogen Phosphate	BrO_3^-	Bromate
CO_3^{2-}	Carbonate	BrO_2^-	Bromite
HCO_3^-	Hydrogen Carbonate**	BrO^-	Hypobromite
ClO^-	Hypochlorite	IO_4^-	Periodate
ClO_2^-	Chlorite	IO_3^-	Iodate
ClO_3^-	Chlorate	IO_2^-	Iodite
ClO_4^-	Perchlorate	IO^-	Hypoiodate
$\text{C}_2\text{H}_3\text{O}_2^-$	Acetate		

i WIZE TIP

Naming ionic compounds that contain polyatomic ions are very similar to the naming of other ionic compounds.

[Name of metal cation] [space] [name of polyatomic anion]

Example:

NaNO_3 is sodium nitrate

! WATCH OUT!

Pay attention to the number of O atoms in a polyatomic ion when naming it!

Example:

$\text{ClO}^- \rightarrow \text{hypochlorite}$

$\text{ClO}^{2-} \rightarrow \text{chlorite}$

$\text{ClO}^{3-} \rightarrow \text{chlorate}$

$\text{ClO}^{4-} \rightarrow \text{perchlorate}$

Note: The charge does not change, but the endings change depending on how many oxygen atoms there are!

****Tip:** If you memorize the number of O atoms and charge for each polyatomic ion with the "ate" ending it will be easy to determine the names of the rest of the polyatomic ions!

Examples:

a) $\text{Sn}(\text{NO}_3)_2$ is _____

b) KNO_2 is _____

Naming Covalent Compounds

Covalent bonds are formed between two non-metals.

i WIZE TIP

Covalent compounds are usually written from least to most electronegative.

[prefix][name of first element] [space] [prefix] [name of 2nd element with "-ide" ending]

Prefixes are used to describe the number of atoms. See the prefixes in the table below :)

Note: If there is only one atom on the left, we drop the mono prefix.

Examples:

CO is carbon monoxide (the last vowel in the prefix is dropped if the next letter is also a vowel)

CO₂ is carbon dioxide

mono	1
di	2
tri	3
tetra	4
penta	5
hexa	6
hepta	7
octa	8
nona	9
deca	10

Example:

N₂O₄ is _____

Example: Providing Chemical Formulae and Names for Ionic Compounds

Give a chemical formula for the following compounds:

a) Potassium Fluoride

b) Manganese(II) oxide

c) Ammonium sulfate

Give a name to the following chemical compounds:



Example: Naming Covalent Compounds

a) NF_3

b) CF_4

c) N_2O

1.18.4

Example: Naming Ionic and Covalent Compounds

First state whether each compound is ionic or covalent then name it!



1.18.5

Practice: Naming

What is the name of the chemical compound: $\text{Co}_2(\text{SO}_3)_3$?

Cobalt sulfate

Cobalt(III) sulfate

Cobalt(III) sulfite

Cobalt(II) sulfate

Cobalt(II) sulfite

1.19 Introductory Nomenclature

1.19.1

Types of Formula and Compounds

Definitions:

- Empirical Formula - Tells us the ratio of elements in the molecule
 - Ex. Ethanol C_2H_6O
 - Ex. Acetic Acid CH_3COOH
- Molecular Formula - Tells us the number of and type elements in the molecule. Could be the same as the empirical formula
 - Ex. Ethanol C_2H_6O
 - Ex. Acetic Acid CH_3COOH
- Structural Formula - Tells us the connectivity of the molecule
 - Ex. Ethanol CH_3CH_2OH
 - Ex. Acetic Acid CH_3COOH

Types of Compounds:

- Organic Compounds: Compounds which contain a C-H bond. Typically they are primarily made up of Carbon and Hydrogen but can have small numbers of **heteroatoms** like N, O, S, Cl, Br, I
 - Ex. CH_3CH_2Br
 - Ex. C_6H_5OH
- Inorganic Compounds: Compounds which are not organic....
 - Ex. $NaBr$
 - Ex. PF_5
 - Ex. CO_2

Oxidation States

Definition:

A counting method used to describe the number of electrons lost or gained by an atom

Oxidation State Rules

1. Free elements: oxidation state = 0
2. Monoatomic ions: oxidation state = ionic charge
3. Hydrogen: oxidation state = +1

Exception: hydrogen in hydrides (e.g., NaH) – oxidation state = -1

4. Oxygen: oxidation state = -2
 - a. Exception: oxygen in peroxides (e.g., H₂O₂) – oxidation state = -1

1.19.3

List the oxidation state for each atom in the hydroxide ion (OH^-)

1.19.4

Choose the option below that completes the following sentence correctly.

The oxidation states of the sulphur atom in SO_4^{2-} and SO_3^{2-} are _____ and _____ respectively.

+2, +2

+6, +6

+8, +6

-2, -2

+6, +4

1.19.5

What is the oxidation state of the central carbon atom in CH_4 ?

+4

-4

0

+2

-2

1.20 Organic Nomenclature

1.20.1

A More Detailed Look at Functional Groups

To study organic chemistry in a systematic way we need to be able to look at a molecule and find common fragments (called functional groups) which we can then generalize to all organic molecules.



WIZE CONCEPT

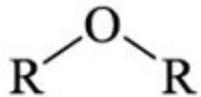
Functional group identification is crucial for naming an organic molecule.

The **functional groups** you are responsible for are shown below along with their **abbreviation** and **priority**.

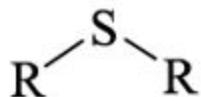
Note: "SN" in the table below is the name you use when that functional group is not highest priority but is a substituent

Carboxylic Acid $\text{R}-\text{C}(=\text{O})-\text{OH}$ Priority 1 $-\text{COOH}$ SN: -carboxyl	Ester $\text{R}-\text{C}(=\text{O})-\text{OR}'$ Priority 2 $-\text{COOR}'$ SN: -oxycarbonyl	Acyl Halide $\text{R}-\text{C}(=\text{O})-\text{X}$ Priority 3 $-\text{COOC}\text{I}$ SN: -halomethanoyl	
Amide $\text{R}-\text{C}(=\text{O})-\text{NR}_2$ Priority 4 $-\text{CONR}_2$ SN: amido	Nitrile $\text{R}-\equiv\text{N}$ Priority 5 $-\text{CN}$ SN: cyano	Aldehyde $\text{R}-\text{C}(=\text{O})-\text{H}$ Priority 6 $-\text{CHO}$ SN: methanoyl	
Ketone $\text{R}-\text{C}(=\text{O})-\text{R}$ Priority 7 RC(O)R SN: oxo	Alcohol $\text{R}-\text{OH}$ Priority 8 $-\text{COH}$ SN: hydroxy	Thiol $\text{R}-\text{SH}$ Priority 9 $-\text{CSH}$ SN: mercaptyl	Amine NR_3 Priority 10 $-\text{NR}_3$ SN: amino

Some other common functional groups are shown below. You will be expected to identify them but they do not have a priority (they have a much lower priority than the functional groups in the table above).



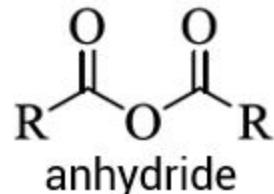
ether



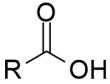
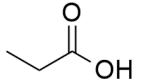
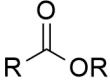
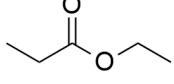
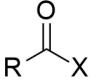
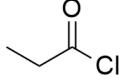
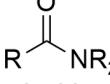
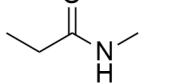
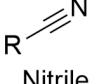
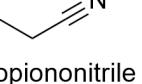
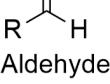
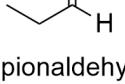
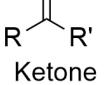
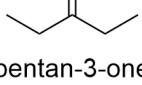
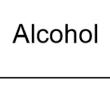
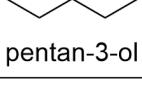
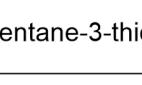
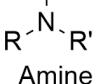
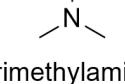
sulfide



alkylhalide



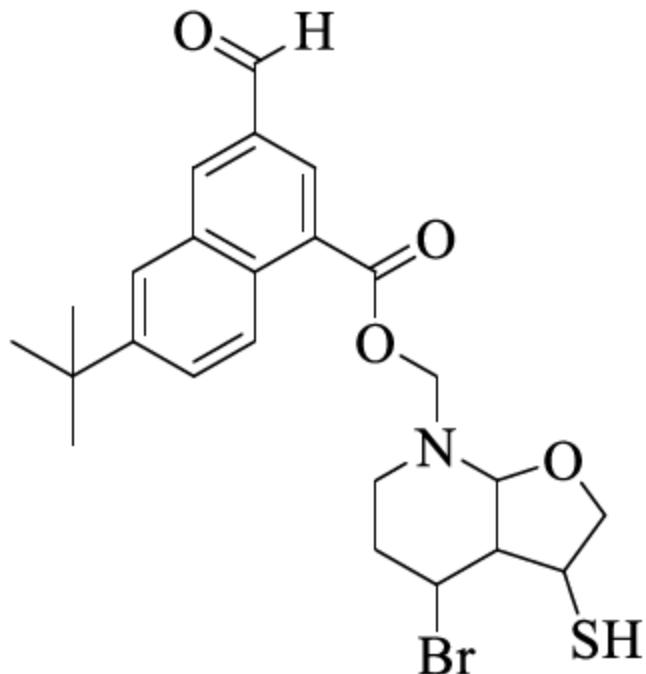
anhydride

Functional Group	Parent Name	Example
 Carboxylic Acid	-oic acid	 propionic acid
 Ester	-oate	 ethyl propionate
 Acyl Halide	-oyl halide	 propionyl chloride
 Amide	-amide	 <i>N</i> -methylpropionamide
 Nitrile	-nitrile	 propiononitrile
 Aldehyde	-al	 propionaldehyde
 Ketone	-one	 pentan-3-one
 Alcohol	-ol	 pentan-3-ol
 Thiol	-thiol	 pentane-3-thiol
 Amine	-amine	 trimethylamine

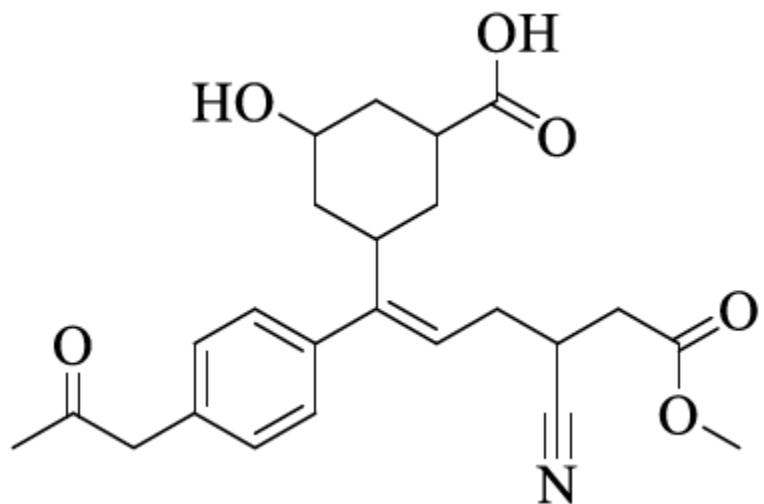
1.20.3

Circle and label all functional groups in the following molecules.

a)



b)



Naming Simple Hydrocarbons

Each name contains:

- A **root** (aka prefix), which tells you how many carbons are in the longest chain
- And a **suffix**, which tells you whether there is a double or triple bond anywhere in the chain

# C's	1	2	3	4	5	6	7	8	9	10
Root	meth	eth	prop	but	pent	hex	hept	oct	non	dec

Type of C – C bond	Suffix
single	ane
double	ene
triple	yne

- If there is a ring simply affix “cyclo” to the beginning of the name
- If there is a double or triple bond (alkene or alkyne) we must designate where in the chain the double bond is located. This is done by placing a number in front of the name.

Example:



non-2-ene
or
2-nonene

non = 9 carbon chain

ene = there is a double bond

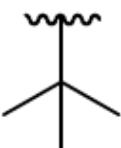
2 = the double bond starts at carbon 2

- If the carbon chain has a branch point, the longest chain becomes the parent molecule and the group coming off becomes a substituent.
 - Substituents use the same root as simple alkanes but the suffix is -yl.

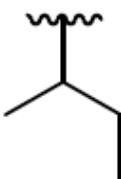
Shown below are a few very common substituents that have non-systematic names.



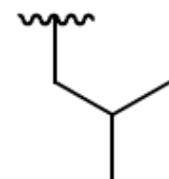
iso-propyl



tert-butyl



sec-butyl



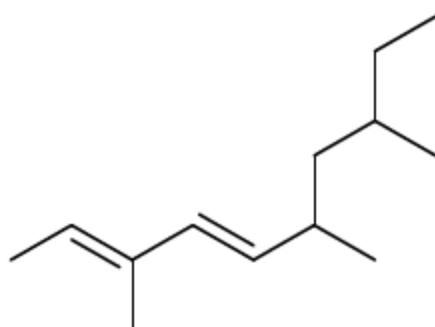
iso-butyl

Steps to Naming Simple Hydrocarbons

1. Identify the **longest carbon chain** and circle it. If the longest carbon chain is a ring then the ring (with no other carbons) becomes the parent. If a ring is a substituent on a larger carbon chain treat it like a substituent (eg. cyclohexyl-)
2. Number the carbon chain so that the **highest priority group** (alkene > alkyne > substituent) has the **lowest possible number**.
3. **List the substituents** with their numbers (which tells you the location on the chain) in **alphabetical order** followed by the root and suffix (with appropriate numbering) of the longest chain.
Note: If the same substituent appears more than once add a prefix of “di” for two “tri” for three, “tetra” for four. These prefixes don’t have to be in alphabetical order
4. Put the stereochemical designation in the very front in brackets.

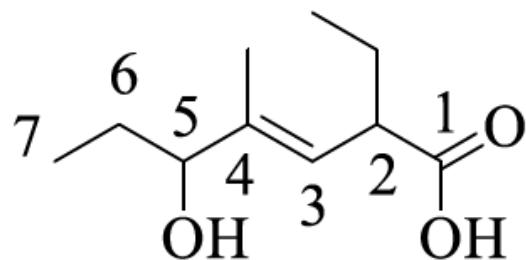
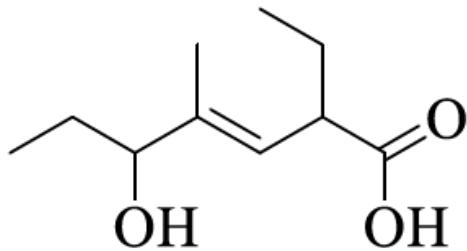
1.20.5

Example: Naming Hydrocarbons



Steps to Naming Complex Organic Molecules

1. Identify all the functional groups and **locate the functional group with highest priority**.
2. **Identify the longest chain** which includes the carbon of the highest priority group.
3. Number the carbons such that the **highest priority functional group has the lowest possible number**
4. **Name the parent chain** with its functional group
5. Add all **substituents alphabetically**
6. Add any stereochemistry (R, S, E, Z) ** Covered Separately **



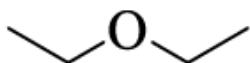
1. The carboxylic acid is the highest priority group
2. The Longest chain that includes the COOH is 7 carbons long
3. Start numbering at the COOH carbon
4. Parent molecule is hept-3-eneoic acid
5. We have one ethyl, one hydroxyl and one methyl so the name becomes:
2 – ethyl – 5 – hydroxyl – 4 – methylhept – 3 – eneoicacid
6. The only stereochemistry indicated is the double bond which is *E* so the name is :

(*E*) –2 – ethyl – 5 – hydroxy – 4 – methylhept – 3 – eneoic acid

Naming Organic Molecules with Odd Functional Groups

- Esters, ethers, sulphides, and amides are weird because they interrupt carbon chains.
- For ethers, sulphides, and amines we name each group coming off as a substituent and place ether, sulphide or amine at the end of the name as shown below.

Ethers

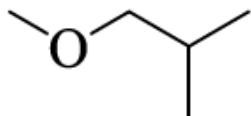


diethylether

Sulfides



dimethylsulfide



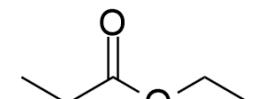
iso-butyl(methyl)ether



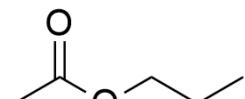
ethyl(methyl)sulfide

For esters, the group attached to the oxygen atom becomes the substituent and the carbon of the ester becomes carbon 1, as long as there is no higher priority group.

Esters

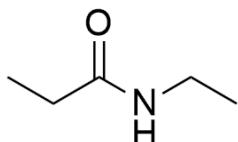


ethyl propionate

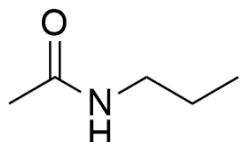


propyl ethionate

Amides



N-ethylpropionamide

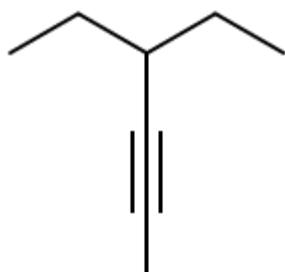


N-propylethionamide

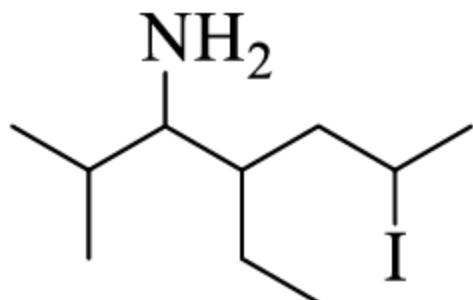
1.20.8

Name the following

a)



b)



1.21

Conformations and Stereochemistry

1.21.1

Conformations and Stereochemistry

Line bond diagrams are excellent ways to quickly show what a molecule looks like. However there are many different ways to draw the same molecule. In this section we will review different projections and look at the way stereochemistry can be identified

- **Stereochemistry:** the study of the spatial arrangement of atoms in molecules.
 - 3-D visualization and spatial skills are key!
- **Stereoisomers:** Two compounds which have identical bond connectivity but differ in their arrangement in 3-D space.

1.21.2

E vs Z

- While single bonds freely rotate at room temperature double and triple bonds do not due to the π bonds. When π double bond is rotated the two p-orbitals which make up the π bond are not adjacent until the rotation is complete, breaking this bond costs energy.



Can alkynes rotate freely at room temperature?

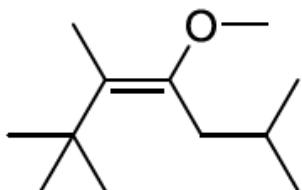
Why Don't we have stereochemical assignments for them?

-
- Due to the lack of rotation about a π bond two stereoisomers are generated shown above. We designate the stereochemistry of double bonds with an E or a Z.
 - E comes from the German word ‘entgegen’ which means opposite
 - Z comes from the German word ‘zusammen’ which means together.

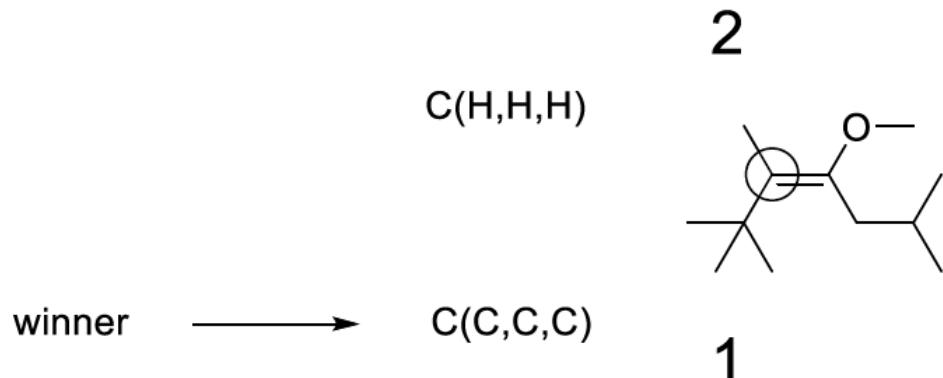
Steps to Assigning E (trans) and Z (cis)

1. Examine each carbon of the double bond and assign the priority of each of the two substituents by atomic weight of the first atom. If the atoms are the same, look at the next atom down the chain. Double bonds count as two single bonds.
2. If the two groups on one end of the alkene are the same and priority cannot be assigned, the alkene has no stereochemistry. E and Z are not required.
3. Examine the priority 1 substituent on each carbon center and determine if they are on the same side (Z) or opposite sides (E)

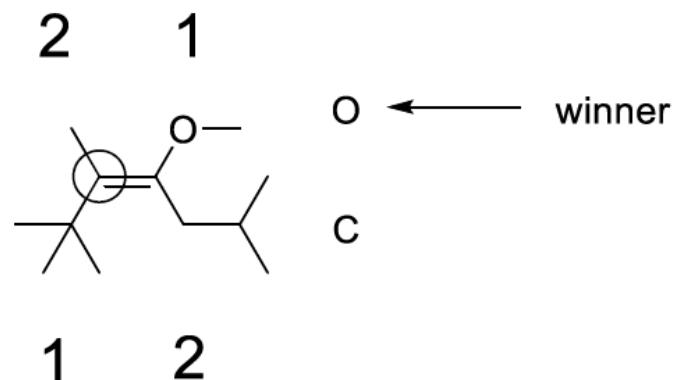
Assign each double bond as E, Z or neither



1. Assign priority on the left end



2. Assign priority on the right end



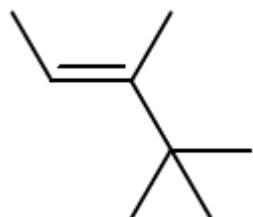
3. Highest priority groups are in opposite sides so this is E

E

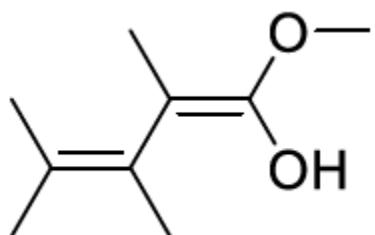
1.21.3

Assign all alkenes in the following molecules as E, Z, or neither.

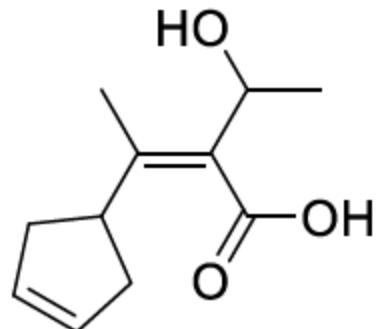
A)



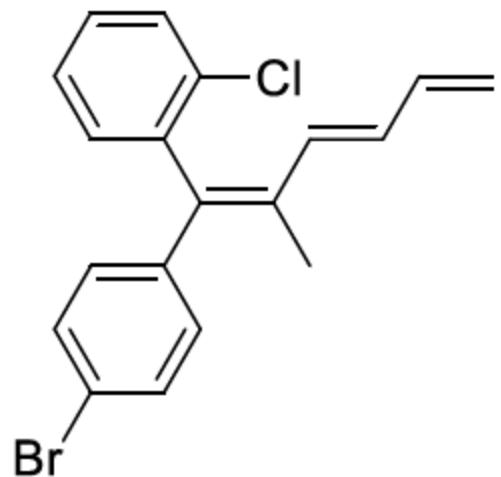
B)



C)



D) Ignore the alkenes in the phenyl ring



1.21.4

Optical Isomers, R vs S

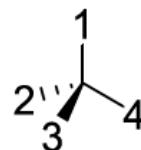
- When four different substituents are attached to a tetrahedral center it is called an asymmetric center.
- If we switch two groups on an asymmetric center the new arrangement is non-superimposable with the original.
- If we switch two groups and the result is non-superimposable we call this a stereocenter. All asymmetric centers are stereocenters!



Non-stereocenter (left) and stereocenter (right)

Steps for Assigning R and S

1. Rank the four substituents based on their priority in the same way as for alkenes. Higher molecular weight atom takes priority, if they are the same element move to the next atom. Double bonds count as two of that bond (C=O is the same as two C-O)
2. Examine the lowest priority group. If it is going back into (dash) the page we have the "correct view", if it is coming out of the page (wedge) we have the "opposite view", if it is in the plane of the page rotate your head so the molecule is in the "correct view".
3. If the priority 1, 2, 3 substituents are arranged in a clockwise fashion it is an R stereocenter, if they are arranged counter clockwise it is S.
4. If you were looking down the "opposite view" switch your assignment. ie. R becomes S and S becomes R.



=



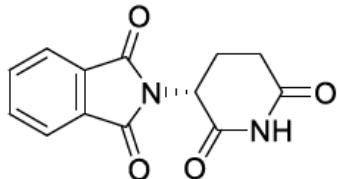
" correct view"

" opposite view"

We have to Rotate our Heads

Different Views of the Same Stereocenter Rotated About the Vertical Axis

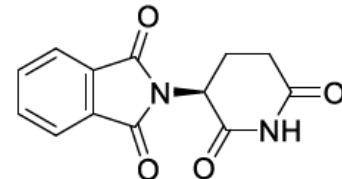
- Enantiomers have the same physical properties but they can react differently to chiral stimuli.
- For example the boiling point, melting point, Gibbs free energy etc. will all be the same for a pair of enantiomers
- However if we shine plane polarized light through a solution of one enantiomer it will rotate the light. We call this its specific rotation.
- If one enantiomer has a (+) rotation of the light the other enantiomer will have a (-) rotation of the same magnitude.
- Another difference happens in the biological world, because our bodies are chiral. Therefore different enantiomers of the same drug can have wildly different properties.



(R)-2-(2,6-dioxopiperidin-3-yl)isoindoline-1,3-dione

(R) - Thalidomide

Causes mild sedation and morning sickness relief



(S)-2-(2,6-dioxopiperidin-3-yl)isoindoline-1,3-dione

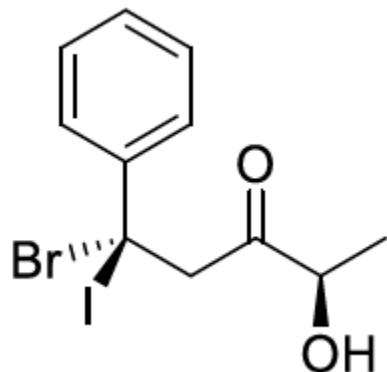
(S) - Thalidomide

Causes extreme birth defects and fetal death

1.21.5

Example: Asymmetric (Chiral) Centres

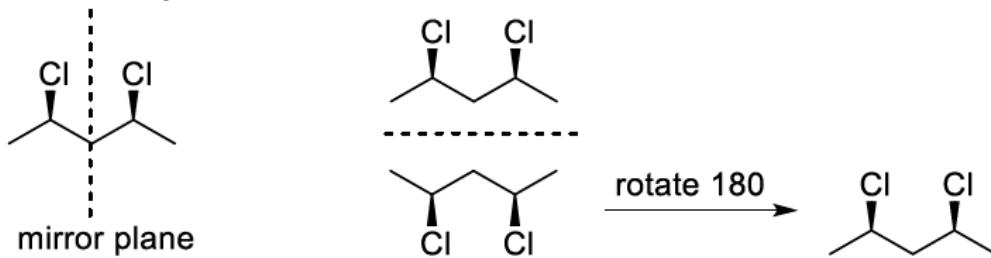
Circle all the asymmetric centers and assign the stereochemistry of each center.



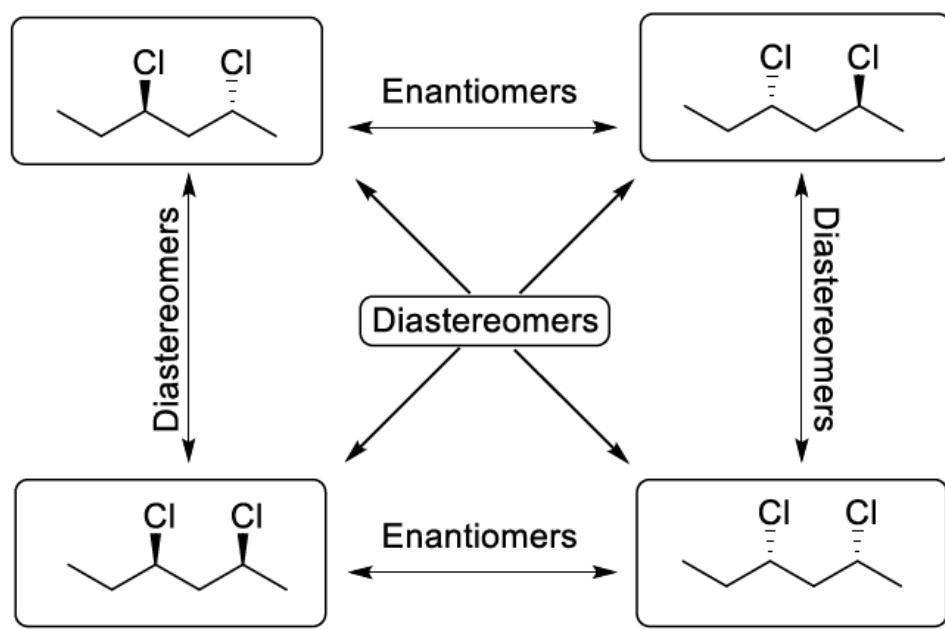
Unrelated vs Diastereomers vs Enantiomers vs Identical

- **Chirality:** A molecule is said to be chiral if its mirror image is **NOT** superimposable.
 - Chiral molecules have chiral centres but cannot possess an internal mirror plane.
- **Enantiomers:** A pair of compounds which are mirror images and **NOT** superimposable
- **Diastereomers:** Stereoisomers which are **NOT** mirror images.
- **Meso compound:** A meso compound is an achiral compound **with an internal mirror plane** which contains chiral centers.
 - The mirror image of a meso compound is identical to the original compound because a meso compound is achiral

Meso Compound



Notice that if we take a chiral molecule with two chiral centers and **change one of the centers** we create a diastereomer but if we **change all the chiral centers** we create an enantiomer.



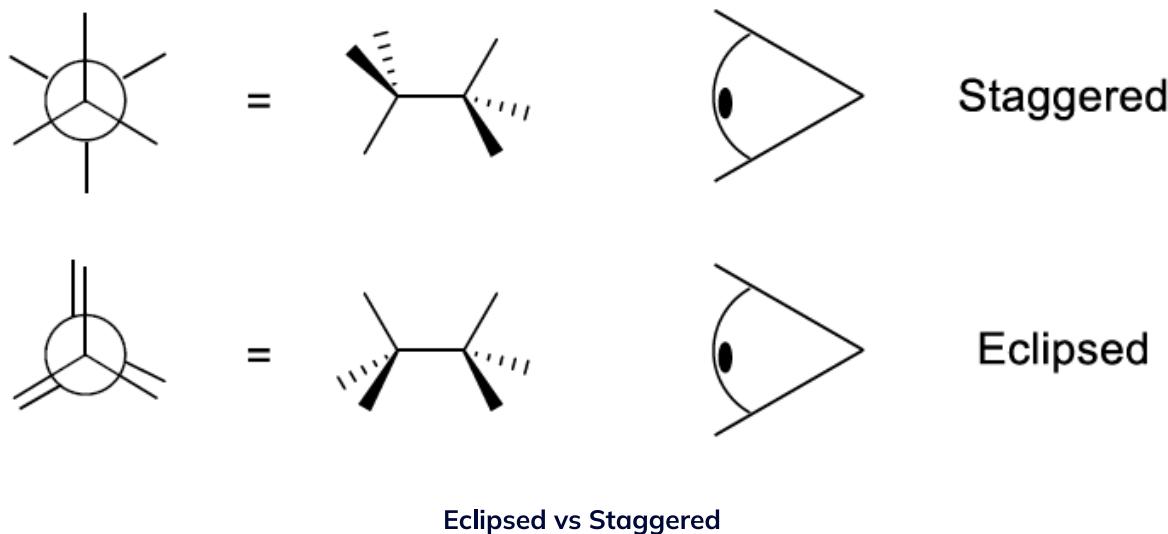
Enantiomers vs Diastereomers

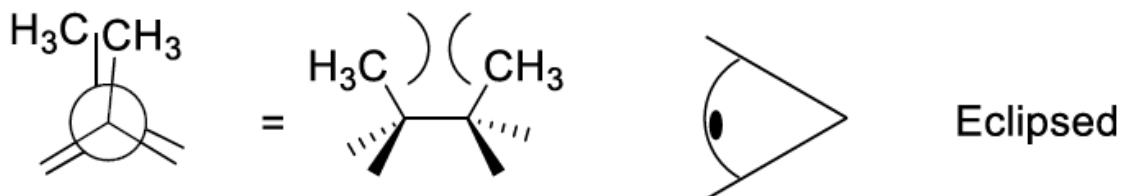
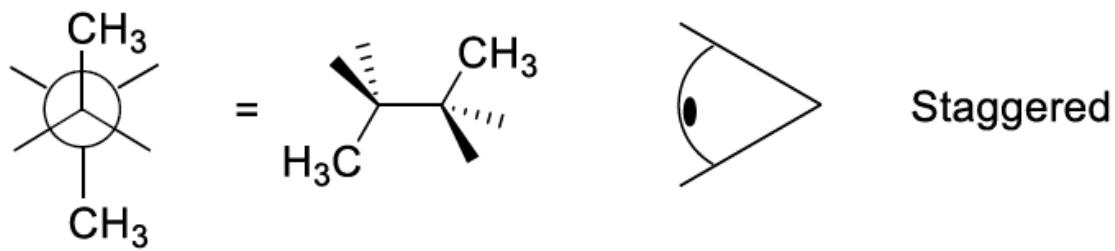
Steps for Identifying Chirality in Molecules

1. Do the molecules have the same bond connectivity?
 - a. If no, they are unrelated compounds
 - b. If yes, move on to step 2
2. Are the compounds superimposable?
 - a. If yes, they are identical
 - b. If no, the molecules are stereoisomers (D or E)
3. Are the compounds mirror images?
 - a. If no, the compounds are diastereomers
 - b. If yes, the compounds are enantiomers

Newman Projections

- A **Newman projection** is drawn by looking down a single bond (typically carbon carbon single bonds) and seeing how substituents on neighbouring carbon atoms are related.
- Once the axis we are looking down is defined, the front carbon is a dot with the three substituents coming out from it. The back carbon is a sphere with its three substituents coming off the sphere.
- **Rotomers:** Isomers which are created by rotating a carbon carbon single bond.





Eclipsed vs Staggered & Steric interactions in Eclipsed Conformation

WIZE CONCEPT

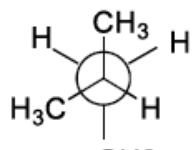
The **eclipsed** geometry is much **higher in energy** because of the steric repulsion between neighboring substituents.

In a staggered geometry we can have our largest groups be **anti** (like the CH₃ above) or **gouche** (where the CH₃ groups are beside on another)

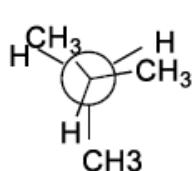
1.21.8

Example: Ranking Rotomers from Lowest to Highest Energy

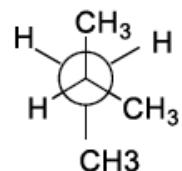
Rank the following rotomers of 2-methylbutane from lowest to highest energy.



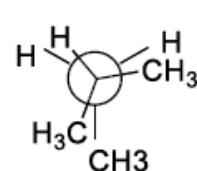
1



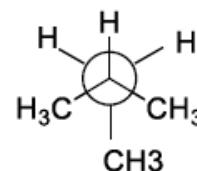
2



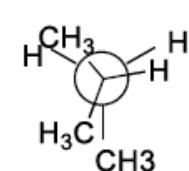
3



4



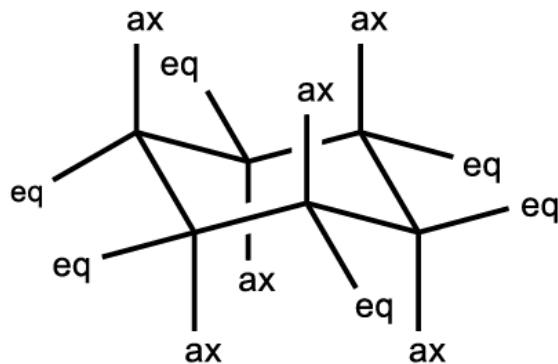
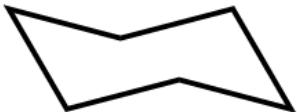
5



6

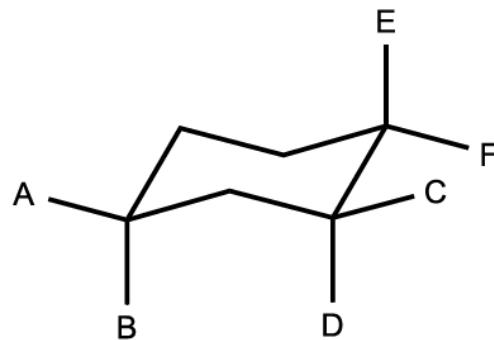
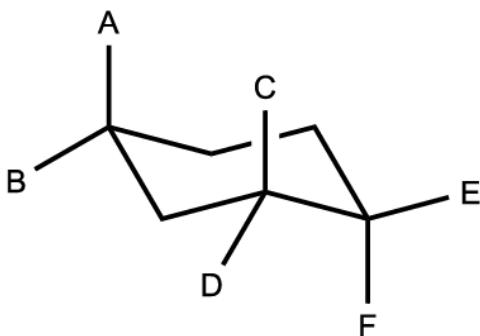
Cyclohexane Rings

- Cyclohexane rings are not planar, even though we sometimes draw them that way.
- Cyclohexane rings usually adopt a chair like shape.
- The chair, shown below, has 6 tetrahedral carbons in a chair like shape; each carbon has one axial and one equatorial substituent. The axial substituents alternate whether they are pointing up or down.



Axial and Equatorial Substituents

- Cyclohexane rings can undergo “ring-flip” as shown below. In the process, all groups that were equatorial become axial and all the axial groups become equatorial.

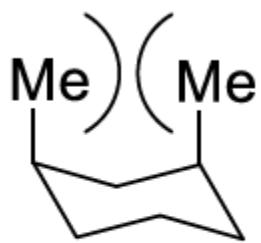


Ring Flip

- Notice that A is still above B C is still above C and E is still above F. The only change is which is axial and which is equatorial. This allows us to easily represent chairs as line drawings.

Stability of Chair Conformers

- If we compare the two ring-flip conformers we can determine which of the two conformers is more stable based on the position of the largest group.
- The conformer which places the largest group in an equatorial position will be more stable because the steric repulsion will be less



Less Stable



More Stable

Stability of Chair Conformers