Atoms, Molecules and Ions

Chapter 2 and Chapter 3 (3.1, 3.2) "Chapter 2 Part 2"

Chemistry 221
Professor Michael Russell

MAR Last update: 4/10/23



Early chemists describe the first dirt molecule

Poor Auntie Jane!

Auntie Jane fed Baby Nell What she thought was calomel What the baby really ate

was Corrosive Sublimate

Not much difference, I confess.

Just one chlorine more

and one baby less!

calomel = HgCl (for dysentery) Corrosive Sublimate = $HgCl_2$





Molecules, lons and Compounds Ozone, 03 NaCl, salt Buckyball, C₆₀ Methane, CH₄

Compounds and Molecules

COMPOUNDS are a combination of 2 or more elements in definite ratios by mass.

The character of each element is lost when forming a compound.

MOLECULES are the smallest unit of a compound that retains the characteristics of the compound.



MAR

MOLECULAR FORMULA

Formula for glycine is $C_2H_5NO_2$ In one molecule there are

2 C atoms

5 H atoms

1 N atom

2 O atoms



Writing Formulas

Can also write glycine formula ($C_2H_5NO_2$) as H_2NCH_2COOH

to show atom ordering

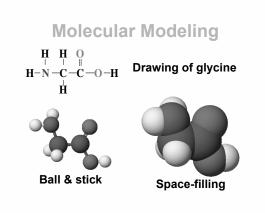
or in the form of a Structural formula

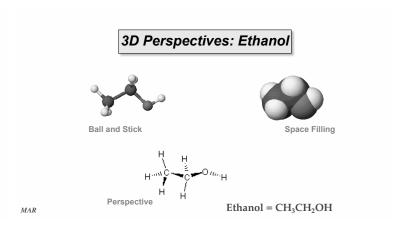


MAR

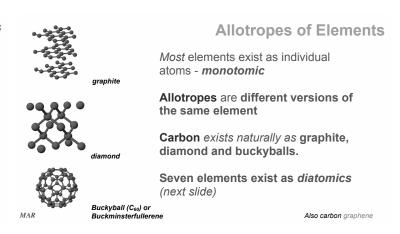
structural formulas also called "condensed" formulas

MAR





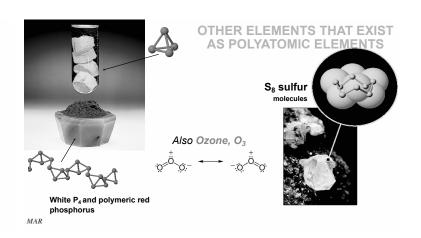
	Comparison of Formula Types		
Compound	Molecular	Empirical	Structural
Water	H_2O	H_2O	нон
Hydrogen Peroxide	H_2O_2	но	ноон
Ethylene	C_2H_4	CH_2	H ₂ CCH ₂
Ethane	C_2H_6	CH ₃	H ₃ CCH ₃
Ethanol	C_2H_6O	C_2H_6O	H ₃ CCH ₂ OH
Dimethyl ether	C_2H_6O	C_2H_6O	H ₃ COCH ₃



Have
No
Fear
Of
Ice
Clear
Brew

Most elements are monatomic - they exist as individual atoms - but there are these seven exceptions:

Nitrogen, N2



MAR

MAR

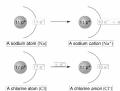
IONS AND IONIC COMPOUNDS

IONS are atoms or groups of atoms with a positive or negative charge.

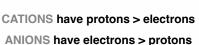
Taking away electron(s) creates a CATION with a positive charge

Adding electron(s) creates an ANION with a negative charge.



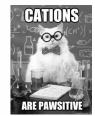


IONS AND IONIC **COMPOUNDS**





CATS have PAWS CATions are PAWSitive



MAR

MAR

Formation of Cations and Anions

Cation

Mg --> Mg2+ + 2 e-

A cation forms when an atom loses one or more electrons.

F + e- --> F-

An anion forms when an atom gains one or more electrons

Charges on Metals

Fixed charge metals include:

*Groups IA, IIA & "stairs" (next slide) *charge = group number (mostly)

sodium ion Na+ Mg²⁺ magnesium ion **AI**3+ aluminum ion silver ion Ag+

All other metals ("variable charge" metals) --> use Roman number to represent charge on metal

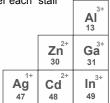
Fe2+ iron(II) ion Fe3+ iron(III) ion MAR V3+ vanadium(III) ion

No ferrous or ferric nomenclature!

The Fixed Charge "Stairs" Metals

- Start with AI (which is +3)
- · Go backwards down the "stairs"

• Decrease charge after each "stair"



These, and Groups IA and IIA, are the "fixed charge metals", and we always know their ionic charge NONMETALS

NONMETAL + n e- ----> Xnwhere charge = Group no. - 8



webelements.com: group no. - 18 Group 5A Group 6A C4-,carbide N³⁻, nitride O2-, oxide F-, fluoride S2-, sulfide Cl-, chloride Name derived Br-, bromide I-, iodide

by adding -ide to stem

MAR

A "Quick and Dirty" Guide to Ionic Charges

Groups IA, IIA or "the stairs": fixed charge metals
Charge = positive
Magnitude = group # mostly!

Groups VA, VIA or VIIA: fixed charge nonmetals
Charge = negative
Charge = group # - 8

All Other Metals: Difficult to predict, use Roman number to represent positive charge, these are the "Variable Charge metals"

POLYATOMIC IONS

Groups of atoms with a charge.

MEMORIZE the names and formulas in your text and the "Nomenclature" lab.



Charge	Formula	Name	Formula	Name
1-	H-	Hydride ion	CH ₃ COO ⁻ (or C ₂ H ₃ O ₂ ⁻)	Acetate ion
	F-	Fluoride ion	CIO ₃	Chlorate ion
	CI	Chloride ion	CIO ₄	Perchlorate ion
	Br ⁻	Bromide ion	NO ₁	Nitrate ion
I CN	Ι"	Iodide ion	MnO ₄	Permanganate ion
	CN-	Cyanide ion		
	OH-	Hydroxide ion		
2- O ²⁻ O ₂ ²⁻ S ²⁻	O ²⁻	Oxide ion	CO ₂ 2-	Carbonate ion
	O ₂ 2-	Peroxide ion	CrO ₄ 2-	Chromate ion
	S2-	Sulfide ion	Cr ₂ O ₂ 2-	Dichromate ion
		CO ₃ ²⁻ CrO ₄ ²⁻ Cr ₂ O ₇ ²⁻ SO ₄ ²⁻	Sulfate ion	
3-	N ³	Nitride ion	PO ₄ 3	Phosphate ion

MAR

Formula	Name	Formula	Name	
CATION: Positive Ion				
NH ₄ ⁺	ammonium ion			
ANIONS: Negative Ions				
Based on a Group 4A element	Based on a Group 4A element		Based on a Group 7A element	
CN-	cyanide ion	CIO-	hypochlorite ion	
CH3CO2-	acetate ion	ClO ₂ -	chlorite ion	
CO32-	carbonate ion	CIO3-	chlorate ion	
HCO ₃ -	hydrogen carbonate ion	CIO ₄ -	perchlorate ion	
	(or bicarbonate ion)			
Based on a Group 5A element		Based on a tro	ansition metal	
N0 ₂ -	nitrite ion	Cr0₄²−	chromate ion	
NO ₃ -	nitrate ion	Cr ₂ 0 ₇ 2-	dichromate ion	
P043-	phosphate ion	MnO ₄ -	permanganate ion	
HPO ₄ 2-	hydrogen phosphate ion		· ·	
H ₂ PO ₄ -	dihydrogen phosphate ion	Note: many O containing anions have names ending in		
Based on a Group 6A element				
OH-	hydroxide ion			
50 ₂ e-	sulfite ion			
50 ₄ 2-	sulfate ion	-ate (or -	ite).	
HSO ₄ -	hydrogen sulfate ion	(,	
•	(or bisulfate ion)			

Introducing: Nick the Camel!
Nick the Camel Brat ate Icky Clam for Supper in Phoenix



MAR

Nick the Camel

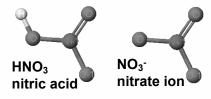
Nick the Camel Brat ate Icky Clam for Supper in Phoenix

Consonants =		Vowels =	Polyatom	
		Oxygen _	Charge	Ion
	Nick = Nitrate	3	-1	NO ₃ -
	\underline{C} amel = C arbonate	3	-2	CO ₃ 2-
	<u>Br</u> at = Bromate	3	-1	BrO ₃ -
	<u>I</u> cky = Iodate	3	-1	IO ₃ -
	<u>Cl</u> am = Chlorate	3	-1	CIO ₃ -
	<u>Supper = Sulfate</u>	4	-2	5O ₄ ²⁻
	Phoenix = Phosphate	4	-3	PO ₄ 3-

Did Nick have Crepes for dessert too? :)

 \underline{Cr} epes = chromate 4 -2 CrO_4 2-

Some Common Polyatomic Ions



Many polyatomic ions related by a hydrogen ion (H+) to an acid

Potassium nitrate somewhat common!

MAR

MAR

MAR

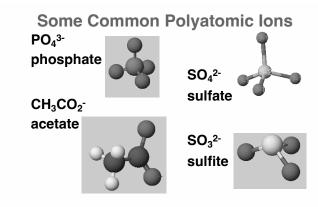
MAR

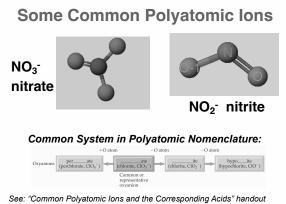
Some Common Polyatomic Ions NH₄+ is the ammonium ion One of the few common polyatomic cations ammonia (NH₃) plus acid (H+) gives the ammonium cation:

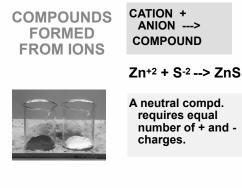
MAR

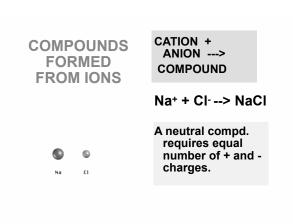
MAR

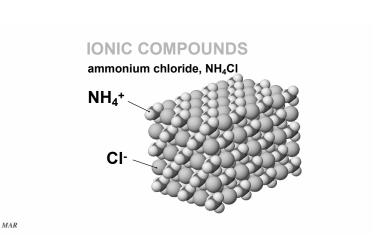
MAR











Page III-2b-5 / Chapter Two Part II Lecture Notes

Some Ionic Compounds

Ca2+ + F- --->

CaF₂

Name = calcium fluoride

Mg²⁺ + NO₃- ---->

 $Mg(NO_3)_2$

Name = magnesium nitrate

Fe²⁺ + PO₄³⁻ ---->

calcium fluoride

Fe₃(PO₄)₂

Name = iron(II) phosphate
also: FePO₄ Name = iron(III) phosphate,

etc.

MAR

MAR

Properties of Ionic Compounds Forming NaCl from Na and Cl₂



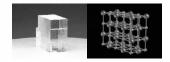
A metal atom can transfer an electron to a nonmetal.

The resulting cation and anion are attracted to each other by

electrostatic forces.

Na

Electrostatic Forces



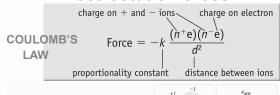
The oppositely charged ions in ionic compounds are attracted to one another by ELECTROSTATIC FORCES.

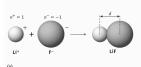
These forces are governed by COULOMB'S LAW.

MAR

MAR

Electrostatic Forces









charge on + and - ions charge on electron COULOMB'S Force = $-k \frac{(n^+e)(n^-e)}{d^2}$ proportionality constant distance between ions

As ion charge increases, the attractive force

As the distance between ions increases, the attractive force _____.

This idea is important and will come up many times in future discussions - see handout

Importance of Coulomb's Law



NaCl, Na⁺ and Cl⁻, m.p. 804 °C



MgO, Mg²⁺ and O²⁻ m.p. 2800 °C

MAR

Molecular (Covalent) Compounds Compounds without Ions





NO₂ nitrogen dioxide



CO₂ carbon dioxide





CH₄ methane

BCI₃ boron trichloride

Naming Molecular (Covalent) Compounds





CO₂ Carbon dioxide

Covalent compounds formed from two or more nonmetals; use **Greek prefixes**





boron trichloride

Ionic compounds generally involve a metal and nonmetal (NaCl) - do not use Greek prefixes with metals!

Greek Prefixes

MAR

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



Three Types of Compound Naming

Fixed charge metal + nonmetal (ionic) No Greek prefixes or Al₂O₃ - aluminum oxide

Variable charge metal + nonmetal (ionic)
Use Roman numbers Fe₂O₃ - iron(III) oxide

Watch variable charge: FeO = iron(II) oxide, etc.

Nonmetal + nonmetal (covalent) Use Greek prefixes P₂O₃ - diphosphorus trioxide

Also P_2O_5 , = diphosphorus pentoxide, etc.

ACIDS

Acids create hydrogen ions in water, acidic H+ listed first in compound

more in Chapter Four and Nomenclature Lab

Some acids include:

HCI hydrochloric HNO_3 nitric **HCIO**₄ perchloric H₂SO₄ sulfuric



HBrO hypobromous BASES

Bases are metal hydroxides, creating OH- in water

Some bases include:

NaOH sodium hydroxide **KOH** potassium hydroxide LiOH lithium hydroxide calcium hydroxide Ca(OH)₂ Fe(OH)₃ iron(III) hydroxide

more in Chapter Four and Nomenclature Lab MAR

Hydrated Compounds

When prepared in water and isolated as solids, many ionic compounds have water molecules trapped in the lattice.

"Waters of hydration" result in beautiful colors

 $CuSO_4.5 H_2O_{(s)} + heat$ $\rightarrow CuSO_{4(s)} + 5 H_2O_{(q)}$



Hydrated Compounds

Nomenclature: use Greek prefix + "hydrate" after regular name

CuSO₄·5 H₂O = copper(II) sulfate pentahydrate MgSO₄·7 H₂O = magnesium sulfate heptahydrate NiCl₂·6 H₂O = nickel(II) chloride hexahydrate

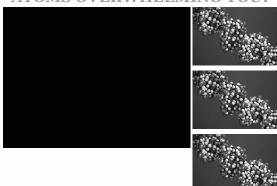
CuSO₄ without water called "anhydrous" copper(II) sulfate

y canate



MAR

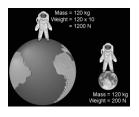
ATOMS OVERWHELMING YOU?



MOLECULAR WEIGHT AND MOLAR MASS

Molecular weight is the sum of the atomic weights of all atoms in the molecule.

Molar mass = molecular weight in grams



MAR

What is the molar mass of ethanol, C_2H_6O ?



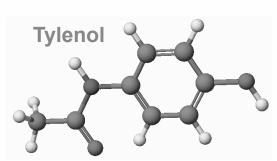
1 mol contains

2 mol C (12.01 g C/1 mol) = 24.02 g C

6 mol H (1.01 g H/1 mol) = 6.06 g H

1 mol O (16.00 g O/1 mol) = 16.00 g O

TOTAL = molar mass = 46.08 g/mol



Formula = C₈H₉NO₂ Molar mass = 151.16 g/mol

MAR

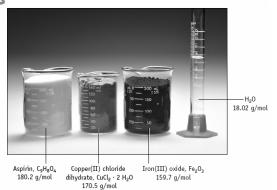
MAR

MAR

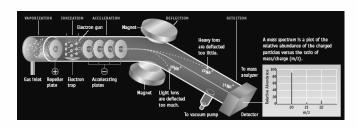
Molar Mass

MAR

MAR



How to Determine a Formula?



Mass spectrometer

Mass Spectrum of Ethanol (NIST) 100. 80. CH₂O31 CH₃CH₂O45 CH₃CH₂O45 Molar mass = 46.08 g mol⁻¹

How many moles of alcohol (ethanol) are present in a "standard" can of beer if there are 21.3 g of C_2H_6O ?

- (a) Molar mass of $C_2H_6O = 46.08$ g/mol
- (b) Calc. moles of alcohol

21.3 g •
$$\frac{1 \text{ mol}}{46.08 \text{ g}} = 0.462 \text{ mol}$$

How many molecules of alcohol (ethanol) are present in a "standard" can of beer if there are 21.3 g of C_2H_6O ?

We know there are 0.462 mol of C₂H₆O.

$$0.462 \text{ mol} \bullet \frac{6.022 \times 10^{23} \text{ molecules}}{1 \text{ mol}}$$

= 2.78 x 10²³ molecules

2.78216...E23

How many atoms of C are present in a "standard" can of beer if there are 21.3 g of C_2H_6O ?

We know there are 2.78 x 10²³ molecules. Each molecule contains 2 C atoms. Therefore, the number of C atoms is

2.78 x
$$10^{23}$$
 molecules • $\frac{2 \text{ C atoms}}{1 \text{ molecule}}$

= 5.56 x 10²³ C atoms

5.56E23

 $2.78 *10^{23} * 9 = 2.50 \times 10^{24}$ atoms in the 21.3 g of ethanol!

MAR

Empirical and Molecular Formulas

A pure compound always consists of the same elements combined in the same proportions by weight.

Therefore, we can express molecular composition as PERCENT BY WEIGHT

Ethanol, C₂H₆O 52.13% C, 13.15% H, 34.72% O

MAR

MAR



Percent Composition

Consider the nitrogen-oxygen family of compounds:

NO₂, nitrogen dioxide, and NO, nitrogen monoxide (or *nitric oxide*)





Structure of NO₂

Chemistry of NO, nitrogen monoxide

Percent Composition

Consider NO₂, Molar mass = ? What is the weight percent of N and of O?

To find the weight percent of an element in a compound:

Wt. %
$$X = \frac{g \text{ of } X \text{ in compound}}{\text{molar mass of compound}} \bullet 100\%$$

In water (H₂O).

Wt. % O =
$$\frac{16.00 \text{ g O}}{18.02 \text{ g H}_2\text{O}} \bullet 100\% = 88.79 \%$$

%H = 100 - 88.79 = 11.21% MAR

Percent Composition

Consider NO₂, Molar mass = ? What is the weight percent of N and of O?

Wt. % N =
$$\frac{14.01 \text{ g N}}{46.01 \text{ g NO}_2} \bullet 100\% = 30.45 \%$$

Wt. % O =
$$\frac{2(16.00 \text{ g O})}{46.01 \text{ g NO}_2} \bullet 100\% = 69.55 \%$$

Test yourself: What are the weight percentages of N and O in N_2O_4 ?

Determining Formulas

In chemical analysis we first determine the % by weight of each element in a given amount of pure compound and derive the EMPIRICAL or SIMPLEST formula.

Weight percentages lead to empirical formulas (but not molecular formulas!)

PROBLEM: A compound of B and H is 81.10% B. What is its empirical

formula?

A compound of B and H is 81.10% B. What is its **empirical** formula?

Calculate the number of moles of each element in 100.0 g of sample.

81.10 g B •
$$\frac{1 \text{ mol}}{10.81 \text{ g}} = 7.502 \text{ mol B}$$

18.90 g H •
$$\frac{1 \text{ mol}}{1.008 \text{ g}} = 18.75 \text{ mol H}$$

MAR

A compound of B and H is 81.10% B. What is its empirical formula?

Take the ratio of moles of B and H. Always

divide by the smaller number.

$$\frac{18.75 \text{ mol H}}{7.502 \text{ mol B}} = \frac{2.499 \text{ mol H}}{1.000 \text{ mol B}} = \frac{2.5 \text{ mol H}}{1.0 \text{ mol B}}$$

But we need a whole number ratio.

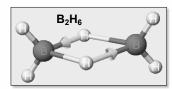
2.5 mol H/1.0 mol B = 5 mol H to 2 mol B

EMPIRICAL FORMULA = B_2H_5

MAR

The compound has an empirical formula of B₂H₅. What is its molecular formula?

Is the molecular formula B₂H₅, B₄H₁₀, B₆H₁₅, B₈H₂₀, etc.?



B₂H₆ is one example of this class of compounds.

The compound has an empirical formula (EF) of B2H5. What is its molecular formula?

To solve, need the molar mass of the compound using a mass spectrometer (a separate experiment)

Next, determine molar mass of the empirical formula

Compare molar mass of the compound to the molar mass of the empirical formula to get a whole number ratio of empirical formula units in the molecular formula

The compound has an empirical formula (EF) of B2H5. What is its molecular formula?

Example:

A compound has an empirical formula of CH2 and a molar mass of 28.1 g mol-1. Find the molecular formula.

Molar mass compound (28.1 g mol-1) given via outside experiment.

Molar mass empirical formula (CH2) =

Now compare molar mass compound to molar mass of

empirical formula:

$$\frac{28.1 \text{ g/mol}}{14.03 \text{ g/mol of CH}_2} = \frac{2 \text{ units of CH}_2}{1 \text{ mol}}$$

Molecular formula = $(CH_2)_2 = C_2H_4$

The compound has an empirical formula (EF) of B2H5. What is its molecular formula?

In the boron problem,

Molar mass of compound (from mass spectrometer, a separate experiment) = 53.3 g/mol

Molar mass of empirical formula (B_2H_5) = 26.67 g/mol

(2*10.81 + 5*1.01 = 26.67 g/mol of EF)

Now find ratio of these masses.

$$\frac{53.3 \text{ g/mol}}{26.67 \text{ g/mol of } B_2H_5} = \frac{2 \text{ units of } B_2H_5}{1 \text{ mol}}$$

Molecular formula = $(B_2H_5)_2 = B_4H_{10}$

Determining a Molecular Formula: Overview

First, convert percent by mass element values into moles (assume 100 g), then compare the moles to get the empirical formula (EF)

$$\frac{18.75 \text{ mol H}}{7.502 \text{ mol B}} = \frac{2.499 \text{ mol H}}{1.000 \text{ mol B}} = \frac{2.5 \text{ mol H}}{1.0 \text{ mol B}}$$

2.5 mol H/1.0 mol B = 5 H to 2 B = B_2H_5

Next, find the molar mass (MM) of the compound, then compare MM of compound to MM of EF

 $\frac{53.3 \text{ g/mol}}{26.67 \text{ g/mol of } B_2 H_5} = \frac{2 \text{ units of } B_2 H_5}{1 \text{ mol}}$

Molecular formula = $(B_2H_5)_2 = B_4H_{10}$

MAR

Determine the formula of a compound of Sn and I using the following data.

(a) Weighed samples of tin (left) and iodine (right).

MAR







Mass of Sn in the beginning = 1.056 g Mass of iodine (l_2) used = 1.947 g Mass of Sn remaining = 0.601 g

Tin and lodine Compound

Find the mass of Sn that combined with 1.947 g l₂.

Mass of Sn initially = 1.056 g Mass of Sn recovered = 0.601 g Mass of Sn used =

Find moles of Sn used:

$$0.455 \text{ g Sn} \cdot \frac{1 \text{ mol}}{118.7 \text{ g}} = 3.83 \text{ x } 10^{-3} \text{ mol Sn}$$

Tin and lodine Compound

Now find the number of moles of I_2 that combined with 3.83 x 10-3 mol Sn

Mass of I_2 used = 1.947 g

1.947 g
$$I_2 \cdot \frac{1 \text{ mol}}{253.81 \text{ g}} = 7.671 \text{ x } 10^{-3} \text{ mol } I_2$$

But we need **mol of I** for formula, not I_2 , so convert:

$$7.671 \times 10^{-3} \text{ mol } I_2 \bullet \frac{2 \text{ mol } I}{1 \text{ mol } I_2} = 1.534 \times 10^{-2} \text{ mol } I$$

So 1.534 x 10⁻² mol of iodine atoms were used in this reaction

Tin and lodine Compound

Now find the ratio of number of moles of moles of I and Sn that combined.

$$\frac{1.534 \times 10^{-2} \text{ mol I}}{3.83 \times 10^{-3} \text{ mol Sn}} = \frac{4.01 \text{ mol I}}{1.00 \text{ mol Sn}}$$

Empirical formula is Snl₄ tin(IV) iodide

MAR

MAR

End of Chapter 2 Part 2













MAR

Important Equations, Constants, and Handouts from this Chapter:

A mole = 6.022 x 10²³

- · be able to find the molar mass of any compound using the periodic
- be able to convert grams of a compound into moles and/or molecules
- understand how to calculate empirical formula (EF) and molecular formula (MF) using the molar mass and mass percentages

Nomenclature: Greek prefixes, Roman numbers, nonmetal + nonmetal, fixed charge metal + nonmetal, variable charge metal + nonmetal, polyatomic ions, acids, bases, hydrated compounds, the 7 diatomics, cations, anions, covalen ionic, the "stairs", Coulomb's Law

• End of Chapter Problems (following this slide)

See also:

• Chapter Two Part 2 Study Guide Chapter Two Part 2 Concept Guide • Important Equations (following this slide) End of Chapter Problems: Test Yourself

- See practice problem set #3 and self quizzes for nomenclature examples and practice

 1. Determine the molar mass for aluminum chloride, iron(III) oxide and

- Determine the molar mass for aluminum chloride, iron(III) oxide and phosphorus tribromide.
 How many grams in 0.0255 mol of propanol (C₃H₇OH)? How many molecules? How many atoms of C?
 Calculate the weight percent of lead in PbS, lead(II) sulfide. What mass of lead (in grams) is present in 10.0 g of PbS?
 Succinic acid has an empirical formula is C₂H₃O₂ and a molar mass is 118.1 g/mol. What is its molecular formula?
 A new compound containing xenon and fluorine was isolated by shining sunlight on a mixture of Xe (0.526 g) and F- gas. If you isolate 0.678 g of the new compound, what is its empirical formula?
 Direct reaction of iodine (I₂) and chlorine (Cl₂) produces an iodine chloride, I_xCl_y, a bright yellow solid. If you completely used up 0.678 g of iodine and produced 1.246 g of I_xCl_y, what is the empirical formula of the compound? A later experiment showed that the molar mass of I_xCl_y was 467 g/mol. What is the molecular formula of the compound?

End of Chapter Problems: Answers

- 1. 133 g/mol, 160. g/mol, 271 g/mol 2. 1.53 g C₃H₇OH, 1.54 x 10²² molecules, 4.62 x 10²² atoms C 3. 86.59%, 8.66 g Pb 4. C₄H₆O₄ 5. XeF₂ 6. ICl₃, I₂Cl₆

Be sure to view practice problem set #3 and self quizzes for nomenclature examples and practice

MAR MAR