Chapter 2: Atoms, Molecules and Ions

The present picture of the atom has evolved over many hundreds of years. The history of the development of atomic theory is given in your textbook.

These are the 3 fundamental particles given in order of their discovery:

Particle	Mass	Charge	Discoverer
electron (e^-)	0.00055 amu	−1	Davy (1800's) + others
proton (p or p^+)	1.0073 amu	+1	Goldstein (1886)
neutron (n or n^0)	1.0087 amu	0	Chadwick (1932)

In 1910, the research group of Ernest Rutherford ran a most important experiment now called the Rutherford Scattering Experiment, in which a piece of thin gold foil was bombarded with alpha (α) particles (products of radioactive decay).

alpha particle ≡ He nucleus (atom minus its 2 electrons)

$^{4}_{2}He^{2+}$ (it has a 2+ charge)

Most of the positively charged particles passed through the foil (that was expected); but some were deflected by the foil and a few bounced almost straight back. (Surprise!!) What did this mean? (Fig. 5-4, 5-5)

1. atoms are mostly empty space.
2. the mass of an atom is located primarily in the nucleus at the center of the atom.
3. the charge on the nucleus is positive.

Definition of Terms:

atomic number (Z): number of protons in the nucleus
for a neutral atom, ("neutral" means the atom has no charge
the # protons = # electrons so that total charge = 0
the atomic number (# protons) determines an element's identi

2- Extra

Excerpts from Encyclopedia Britannica

Early Atomic Models

Several models of the atom were proposed in the first few years of the 20th century. The earliest (1902) was originated by an English physicist, Lord Kelvin, but was supported so strongly by Thomson that it became known as the Thomson atom. According to this model, the atom consists of a sphere of uniformly distributed positive charge, about one angstrom in diameter (1 angstrom = 10^{-10} m), in which the electrons are embedded like raisons in a pudding. Lord Kelvin himself at least partly abandoned this model and in 1905 proposed another, in which the uniform positive sphere is replaced by alternate positive and negative spherical shells, with a net surplus of positive charge; the electrons are embedded in the positive charge. Another model, proposed in 1903, suggested that all atoms are composed of varying numbers of a single constituent, called dynamids. Each dynamid is conceived as consisting of an intimate association of an electron and a much more massive positive body, having a linear dimension (diameter) of the order of 10^{-4} angstroms with the dynamids held together by unspecified forces. Still another model, proposed in 1904 by a Japanese physicist, Hantaro Nagaoka, considered the positive charge as concentrated at the center of the atom, with the electrons forming a ring similar to Saturn's rings.

The Rutherford Model

In 1910, two researchers working under Rutherford's direction, were studying the scattering of alpha particles - that is, their deflection from straight-line paths - as they passed through thin foils. They noted that a small but significant number were scattered through quite large angles. Rutherford recognized that, if the Thomson model were valid, an alpha particle, about 7000 times more massive than an electron, would interact with many atoms on the way through the foil; no single interaction could produce a large deflection, and the effects of the many interactions would tend to cancel rather than add up. On the other hand, if the positive charge and most of the mass were concentrated in a very small region at the center, as Nagaoka had suggested, multiple interactions would be rare, but a single interaction could produce a large deviation. Rutherford worked out the theory in 1911, that the atom could be described as a tiny, dense, positively charged core called a nucleus, in which nearly all the mass is concentrated, around which the light, negative constituents, called electrons, circulate at some distance, much like planets revolving around the Sun. He showed that the scattering should be proportional to the foil thickness, t, for a nuclear atom but to the square root of the thickness, $\sqrt{t}$, for the Thomson atom; that it should decrease with increasing deflection angle for a nuclear atom but decrease much faster for the Thomson atom. With refined techniques, a complete verification was obtained of the results of the nuclear model, based totally on classical physics. This model did have serious defects: the dynamic equilibrium he proposed, with the electrons travelling around the nucleus, meant, according electromagnetic theory, that the electrons would radiate energy continuously, lose energy and spiral into the nucleus. This does not happen. This problem was resolved by a Danish physicist, Niels Bohr, in 1913, with the Bohr model of the atom.

<u>mass number (A)</u> : sum of numbers of protons and neutrons in the nucleus
therefore, $A = Z$ + no. of neutrons (mass number is <u>not</u> atomic weight)

<u>nuclide symbol</u>

$^{A}_{Z}E$ where E = element symbol
A = mass number (#p + #n)
Z = atomic number (#p)

example : For ^{63}Cu, what is number of protons, electrons, neutrons in ato

ANS. # p = 29 (look on periodic table)
e = 29 (# p = # e for a neutral atom)
n = A − Z = 63 − 29 = 34

<u>isotopes</u> : two or more forms of atoms of the same element with different masses; atoms containing the same number of protons, but different numbers of neutrons.

example: the element hydrogen has 3 isotopes:

hydrogen	deuterium	tritium
$^{1}_{1}H$ (99.985 %)	$^{2}_{1}H$ (0.015 %)	$^{3}_{1}H$ (0.000 %)
1 proton 1 electron 0 neutrons	1 proton 1 electron 1 neutron	1 proton 1 electron 2 neutrons

Some elements have only 1 isotope (F, I), but most elements occur in nature as mixtures of isotopes. The naturally occurring abundances of isotopes (Table 5-3) are determined by mass spectometry

<u>Atomic Weight Scale:</u> 1 amu = $\frac{1}{12}$ mass of ${}^{12}_{6}C$, a specific isotope of C
where amu = atomic mass unit

recall: mass of one ${}^{12}_{6}C$ atom = 12 amu
mass of one mole of ${}^{12}_{6}C$ atoms = $12.000\bar{0}$ g

<u>Atomic Weight of an element</u> : weighted average of masses of its constituent isotopes.

<u>Example</u>: Copper occurs naturally as 2 isotopes

	% abundance	isotopic mass
${}^{63}Cu$	69.1 %	62.9 amu
${}^{65}Cu$	30.9 %	64.9

What is the atomic weight of copper?

$$\text{AW of Cu} = (\text{fraction of } {}^{63}Cu)(\text{mass of } {}^{63}Cu) + (\text{fraction of } {}^{65}Cu)(\text{mass of } {}^{65}Cu)$$
$$= (0.691)(62.9 \text{ amu}) + (0.309)(64.9 \text{ amu})$$
$$= 63.5 \text{ amu}$$

<u>Example</u>: The atomic weight of boron is 10.811 amu. (or look up on periodic table)
The masses of the two isotopes are ${}^{10}B$ 10.013 amu, ${}^{11}B$ = 11.009 amu
What are the % abundances of the 2 isotopes?

let x = fraction of the lighter isotope, ${}^{10}B$
$1-x$ = fraction of the heavier isotope, ${}^{11}B$

$$\text{AW of B} = (\text{fraction of } {}^{10}B)(\text{mass of } {}^{10}B) + (\text{fraction of } {}^{11}B)(\text{mass of } {}^{11}B)$$
$$10.811 = (x)(10.013 \text{ amu}) + (1-x)(11.009 \text{ amu})$$
$$10.811 = 10.013x + 11.009 - 11.009x$$
$$-0.198 = -0.996x$$
$$x = 0.199$$
$$1-x = 0.801$$

$\therefore$ % abundance of ${}^{10}B$ = 19.9 %
${}^{11}B$ = 80.1 %

Atoms and the Mole:

Recall $1\ \text{amu} = \frac{1}{12}$ mass of ^{12}C atom - was an arbitrary decision by scientists

From periodic table

1.0079 amu = mass of an average H atom (weighted average by mass)

22.98977 amu = mass of an average Na atom

therefore ∴ a Na atom has ~ 23 times more mass than a H atom.

Now, atoms are very small, difficult to weigh, difficult to count

So, how do we measure them accurately?

We need a unit which describes a large number of atoms:

mole (SI units) $\text{mol} \equiv 6.022045 \times 10^{23}$ particles
Avogadro's number (N_A)

1 mol Na atoms has 6.022×10^{23} atoms of Na.
(show samples of moles - Fig 2.9)

The system of atomic weights was worked out with N_A so that for an element, atomic weight (in amu) ≡ mass of 1 mol (in grams)

If you look on the periodic table for atomic weight (molar mass) of Na:
you will find 22.98977 or 22.99 (to 4 sig. figures)
∴ if you have 1 atom of Na, it has mass of 22.99 amu
if you have 1 mol of Na atoms, it has mass of 22.99 g.
Pretty amazing!

What about the units?

AW (molar mass) has units of $\frac{\text{grams}}{\text{mol}}$ or $\frac{\text{amu}}{\text{atom}}$

So let's use the units as a formula!

Example: What is the identity of an element if 3.00 moles of it weighs 80.9 g?

Plan: mol, g $\longrightarrow$ A.W. $\longrightarrow$ use periodic table to find identity

atomic weight has units of $\frac{g}{mol}$ – use this as a formula!

$$A.W.\left(\frac{g}{mol}\right) = \frac{\# g}{\# \text{ moles}} = \frac{80.9 \text{ g}}{3.00 \text{ mol}} = 27.0$$

$\therefore$ element must be aluminum, Al

Example: Calculate the mass of an atom of Fe

From periodic table: 1 mol of Fe has mass of 55.85 g
we know 1 mol of Fe contains 6.022×10^{23} atoms

If we combine this information,

$$\underset{(g/atom)}{\text{mass of 1 Fe atom}} = 55.85 \frac{g}{mol} \times \underbrace{\left(\frac{1 \text{ mol}}{6.022 \times 10^{23} \text{ atoms}}\right)}_{\text{UNIT FACTOR}} = 9.274 \times 10^{-23} \frac{g}{atom}$$

Note: this is example of dimensional analysis.

Example: How many moles of atoms and how many atoms are contained in 26.2 g of Fe? (show sample)

(a) $A.W.\left(\frac{g}{mol}\right) = \frac{\# g}{\# \text{ mol}} \Rightarrow \# \text{moles} = \frac{\# g}{AW}$ This is a formula!!

$$\therefore \# \text{moles Fe} = \frac{\# g \text{ Fe}}{AW} = \frac{26.2 \text{ g}}{55.85 \text{ g/mol}} = 0.469 \text{ mol}$$

(b) likewise, we know N_A has units : $\frac{\text{particles}}{\text{mole}}$ $\therefore N_A = \frac{\#\text{ particles}}{\#\text{moles}}$

$$\therefore \#\text{atoms} = N_A \times \#\text{moles}$$
$$= 6.022 \times 10^{23}\ \frac{\text{atoms}}{\text{mol}} \times 0.469\ \text{mol}$$
$$= 2.82 \times 10^{23}\ \text{atoms}$$

Example: How many moles of Hg and how many atoms of Hg are contained in 9.84 mL of Hg (Show vial). Specific gravity of Hg = 13.5939.

we know that $\#\text{moles} = \frac{\#g}{AW}$ but we do not know mass, only volume. What do we know that relates mass and volume? ANS. DENSITY (specific gravity)

density has units $\frac{g}{mL}$ (or $\frac{g}{cm^3}$) $\therefore D = \frac{\#g}{\#mL}$

$$\#g = D \times \#mL$$

$\therefore$ the units of density give you the formula for relating D, mL, g

Recall: specific gravity : ratio of the density of a substance to the density of H_2O (= 1.00 g/mL at 25°C to 3 significant fig)
$\therefore$ for all practical purposes, density ($\frac{g}{mL}$) ≡ specific gravity (no units)

Back to the example:
Plan of attack: $mL \xrightarrow[\text{D or Sp.gr.}]{(1)} g \xrightarrow[AW]{(2)} \text{moles} \xrightarrow[N_A]{(3)} \text{atoms}$

(1) $\#g\ Hg = D \times \#mL$ since $D = \frac{\#g}{\#mL}$
$$= 13.5939\ g/mL \times 9.84\ mL$$
$$= 134\ g$$

(2) $\#\text{ mol Hg} = \frac{\#g}{AW} = \frac{134\ g}{200.59\ g/mol} = 0.668\ \text{mol}$ since $AW = \frac{\#g}{\#mol}$

(3) $\#\text{ atoms} = \#\text{moles} \times N_A$
$$= 0.668\ \text{mol} \times 6.02 \times 10^{23}\ \frac{\text{atom}}{\text{mol}} = 4.02 \times 10^{23}\ \text{atoms}$$
since $N_A = \frac{\#\text{atoms}}{\#\text{mol}}$

Same problem by dimensional analysis:

$$\# \text{atoms Hg} = 9.84 \text{ mL Hg} \times \frac{13.5939 \text{ g}}{1 \text{ mL}} \times \frac{1 \text{ mol}}{200.59 \text{ g}} \times \frac{6.02 \times 10^{23} \text{ atoms Hg}}{1 \text{ mol Hg}}$$
$$= 4.02 \times 10^{23} \text{ atoms Hg}$$

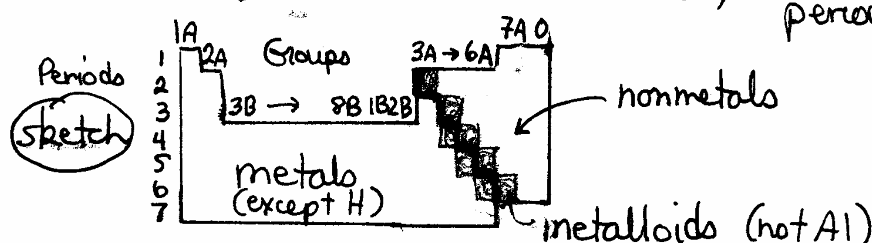
In dimensional analysis, each step is represented by a unit factor

Step 1: converting mL → g
Step 2: converting g → mol
Step 3: converting mol → atoms

Introduction to Periodic Table

- the properties of the elements are periodic functions of their atomic number. (atomic # is # protons in nucleus - and # electrons in a neutral atom)

- Groups or families: vertical columns
  - 1A (except H): alkali metals
  - 2A : alkaline earths
  - 7A : halogens (salt formers)
  - 8A (0) : noble gases – used to be called inert
- Periods: horizontal rows. First row is Period 1.
- Elements can be divided into 3 classes (by staircase division on periodic table.)



- characteristics:

metals	nonmetals
1. high electrical conductivity	1. poor electrical conductivity
2. all are solids (ex. Hg) at room T	2. gases, liquids or solids at room T
3. form cations (+ charged ions) by losing electrons	3. form anions (– charged ions) by gaining electrons
4. form ionic compounds with nonmetals	4. forms covalent cmpds with other non-metals.

(OLD CHAPTER 3 - NOW A PART OF CHAPTER 2)

How do atoms attach themselves to other atoms and how do we name these new compounds?

Two main ways are used to form compounds:

(1) electrons are transferred from one atom to another to form ions.
Ions are held together by electrostatic forces, called ionic bonds.
You easily recognize ionic compounds because they metal cation (+ ion) + nonmetal anion (− on)

Examples: NaCl is really $Na^+ — Cl^-$ (ionic bond)

BaBr$_2$ is really Ba^{2+} — Br^-, — Br^- (Note - not a good picture)

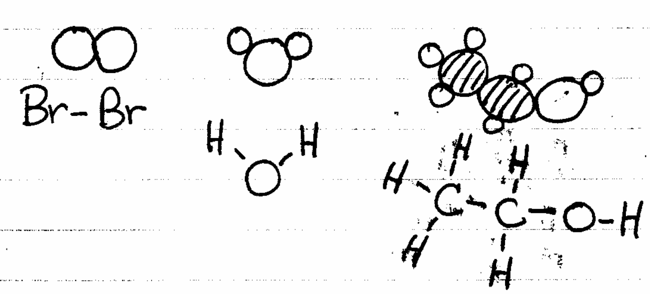
both occur as large lattices

$Cl^- — Na^+ — Cl^- —$
$Cl^- — Na^+ —$
$Na^+ — Cl^-$
$Na^+ — Cl^-$

the final structure has a 1 : 1 ratio between Na^+ and Cl^-. That's why the formula is NaCl. Smallest part is called a <u>formula unit</u>.

(2) electrons are shared between atoms. No ions are formed.
Atoms are held together by forces called covalent bonds.
Covalent compounds are easily recognized because they occur between nonmetals. On the smallest level, the individual units called <u>molecules</u> are formed.

Examples: Br_2 H_2O CH_3CH_2OH



More on ions and ion formation:

the electron is transferred from the Li ~~atom~~ to F atom and LiF is made

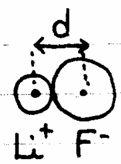
cations (from metals): $\text{Li atom} \rightarrow Li^{+} + e^{-}$
(3p, 3e) (3p, 2e) like He

Note: elements want to have same # e^{-} as noble gases for stability. (more later)

anions (from nonmetals): $\text{F atom} + e^{-} \rightarrow F^{-}$
(9p, 9e) (9p, 10e) ~~like~~ Ne

$$Li + F \longrightarrow Li^{+}, F^{-} \text{ or } LiF$$

the force of attraction, the electrostatic force, called ionic bond is set by Coulomb's Law



$$F \propto \frac{(n^{+} \cdot e)(n^{-} \cdot e)}{d^{2}}$$

$\propto$ is proportional to

n = charge on + or − ion
e = charge on electron
d = distance between ions
F = force

Introduction to Nomenclature for Ionic Compounds:

common cations:

Na^{+}	sodium ion	Cl^{-}	chloride ion
K^{+}	potassium ion	Br^{-}	bromide ion
Ba^{2+}	barium ion	S^{2-}	sulfide ion
Al^{3+}	aluminum ion	N^{3-}	nitride ion

Note: for simple 2 element (binary) ionic compounds <u>only</u>:

1A	+1	2A	+2	3A	+3	metals
5A	−3	6A	−2	7A	−1	nonmetals

name: cation name + anion name – very simple
formula: you must know charges on ions! Relative numbers of ions are adjusted so that total charge of compound is Ø.

sodium nitride $3Na^{+} + N^{3-} \Rightarrow Na_3N$
sodium bromide $Na^{+} + Br^{-} \Rightarrow NaBr$
barium sulfide $Ba^{2+} + S^{2-} \Rightarrow BaS$

Naming Compounds

This is definitely IMPORTANT!

I Binary compounds :

composed of 2 elements
can be ionic or covalent
name less electronegative element first and the more electronegative element second with -ide ending on its stem.

Stems for Nonmetals

IIIA		IVA		VA		VIA		VIIA	
B	bor	C	carb	N	nitr	O	ox	H	hydr
		Si	silic	P	phosph	S	sulf	F	fluor
				As	arsen	Se	selen	Cl	chlor
				Sb	antimon	Te	tellur	Br	brom
								I	iod

A. Binary ionic compounds : contain metal cations and nonmetal anions

KBr : potassium bromide
$CaCl_2$: calcium chloride
NaH : sodium hydride (H is more electronegative - it is anion with -1 charge
EN 1.0 2.1

Mg_3P_2 : magnesium phosphide
Al_2O_3 : aluminum oxide

Metals in binary compounds may exhibit more than one oxidation number. There are 2 ways to express this information.

(1) older method : "-ous" ending for lower oxidation state
"-ic" ending for higher oxidation state

- this only works for those metals with 2 different oxidation numbers.

examples: $\overset{(+1)}{Cu}{}^{+1}$ cuprous $\overset{(+2)}{Fe}{}^{2+}$ ferrous $\overset{(+2)}{Sn}{}^{2+}$ stannous $\overset{(+1)}{Hg_2}{}^{2+}$ mercurous
$\overset{(+2)}{Cu}{}^{2+}$ cupric $\overset{(+3)}{Fe}{}^{3+}$ ferric $\overset{(+4)}{Sn}{}^{4+}$ stannic $\overset{(+2)}{Hg}{}^{2+}$ mercuric

(2) IUPAC method : use roman numeral in parentheses following name

$CuCl_2$ copper(II) chloride (cupric chloride)
Hg_2Br_2 mercury(I) bromide (mercurous bromide)
FeS iron (II) sulfide (ferrous sulfide)

B. Pseudobinary ionic compounds: contain more than 2 elements

cation : NH_4^+ ammonium ion
anion : CN^- cyanide ion
OH^- hydroxide ion

NH_4CN ammonium cyanide
$Sn(OH)_2$ tin (II) hydroxide (stannous hydroxide)

C. Binary Covalent compounds : contains 2 nonmetals
Greek/Latin prefixes give elemental proportions

1. mono (trivial*)	4. tetra	7. hepta	10. deca
2. di	5. penta	8. octa	11. undeca
3. tri	6. hexa	9. nona	12. dodeca

* except for carbon monoxide, CO

SO_2 sulfur dioxide
N_2O_4 dinitrogen tetroxide
As_4O_{10} tetraarsenic decoxide

D. Binary acids : H + more electronegative nonmetal

$HCl(g)$	hydrogen chloride	$HCl(aq)$	hydrochloric acid
$HF(g)$	hydrogen fluoride	$HF(aq)$	hydrofluoric acid
$HI(g)$	hydrogen iodide	$HI(aq)$	hydroiodic acid
$HCN(g)$	hydrogen cyanide	$HCN(aq)$	hydrocyanic acid
$H_2S(g)$	hydrogen sulfide	$H_2S(aq)$	hydrosulfuric acid

II Ternary Compounds

A. Ternary acids (oxyacids) : compounds of H, O, nonmetal

Common ternary acids : "-ic" acids

IIIA	IVA	VA	VIA	VIIA
+3 H_3BO_3 boric acid	+4 H_2CO_3 carbonic acid	+5 HNO_3 nitric acid		
	+4 H_4SiO_4 silicic acid	+5 H_3PO_4 phosphoric acid	+6 H_2SO_4 sulfuric acid	+5 $HClO_3$ chloric acid
		+5 H_3AsO_4 arsenic acid	+6 H_2SeO_4 selenic acid	+5 $HBrO_3$ bromic acid
			+6 H_6TeO_6 telluric acid	+5 HIO_3 iodic acid

there are sets of acids derived from the -ic ternary acids :

1 more O : per____ic acid
1 less O : _____ous acid
2 less O : hypo___ous acid

oxidation state (number) of nonmetal increases ↑			oxidation no. of Cl
per___ic acid	perchloric acid	$HClO_4$	+7
____ic acid	chloric acid	$HClO_3$	+5
____ous acid	chlorous acid	$HClO_2$	+3
hypo__ous acid	hypochlorous acid	$HClO$	+1

B. Ternary Salts: cation (+) or NH_4^+ (ammonium ion) goes first
anion (-) derived from acid goes second

-ic acid	⇒ -ate ion	per___ic acid	⇒ per___ate ion
-ous acid	⇒ -ite ion	hypo___ous acid	⇒ hypo___ite ion

HIO_4	periodic acid	$\xrightarrow{-H^+}$	IO_4^-	periodate ion
HIO_3	iodic acid	$\xrightarrow{-H^+}$	IO_3^-	iodate ion
HIO_2	iodous acid	$\xrightarrow{-H^+}$	IO_2^-	iodite ion
HIO	hypoiodous acid	$\xrightarrow{-H^+}$	IO^-	hypoiodite ion

Note: the charge on the ion can be deduced from the number of Hydrogens on the parent acid.

H_3PO_4	phosphoric acid	$\xrightarrow{-3H^+}$	PO_4^{3-}	phosphate ion
HNO_2	nitrous acid	$\xrightarrow{-1H^+}$	NO_2^-	nitrite ion
H_2SO_4	sulfuric acid	$\xrightarrow{-2H^+}$	SO_4^{2-}	sulfate ion
H_2SO_3	sulfurous acid	$\xrightarrow{-2H^+}$	SO_3^{2-}	sulfite ion
H_2CO_3	carbonic acid	$\xrightarrow{-2H^+}$	CO_3^{2-}	carbonate ion

Examples of salts:

ammonium sulfate	$(NH_4)_2SO_4$
calcium nitrite	$Ca(NO_2)_2$
iron(II) phosphate (ferrous phosphate)	$Fe_3(PO_4)_2$

C. Acid Salts: salts containing an acidic hydrogen or two.

	IUPAC	older name
$NaHSO_4$	sodium hydrogen sulfate	sodium bisulfate
$NaHSO_3$	sodium hydrogen sulfite	sodium bisulfite
KH_2PO_4	potassium dihydrogen phosphate	—
$NaHCO_3$	sodium hydrogen carbonate	sodium bicarbonate

Here is a list of common ions — memorize!

Formulas and Names for Some Common Ions

Common Cations		Common Anions	
Formula	*Name*	*Formula*	*Name*
Li^+	lithium ion	F^-	fluoride ion
Na^+	sodium ion	Cl^-	chloride ion
K^+	potassium ion	Br^-	bromide ion
NH_4^+	ammonium ion	I^-	iodide ion
Ag^+	silver ion	OH^-	hydroxide ion
		CN^-	cyanide ion
Mg^{2+}	magnesium ion	ClO^-	hypochlorite ion
Ca^{2+}	calcium ion	ClO_2^-	chlorite ion
Ba^{2+}	barium ion	ClO_3^-	chlorate ion
Cd^{2+}	cadmium ion	ClO_4^-	perchlorate ion
Zn^{2+}	zinc ion	* CH_3COO^-	acetate ion
Cu^{2+}	copper(II) ion or cupric ion	* MnO_4^-	permanganate ion
Hg_2^{2+}	mercury(I) ion or mercurous ion	NO_2^-	nitrite ion
Hg^{2+}	mercury(II) ion or mercuric ion	NO_3^-	nitrate ion
Mn^{2+}	manganese(II) ion	* SCN^-	thiocyanate ion
Co^{2+}	cobalt(II) ion		
Ni^{2+}	nickel(II) ion	O^{2-}	oxide ion
Pb^{2+}	lead(II) ion or plumbous ion	S^{2-}	sulfide ion
Sn^{2+}	tin(II) ion or stannous ion	HSO_3^-	hydrogen sulfite ion or bisulfite ion
Fe^{2+}	iron(II) ion or ferrous ion		
		SO_3^{2-}	sulfite ion
Fe^{3+}	iron(III) ion or ferric ion	HSO_4^-	hydrogen sulfate ion or bisulfate ion
Al^{3+}	aluminum ion		
Cr^{3+}	chromium(III) ion or chromic ion	SO_4^{2-}	sulfate ion
		HCO_3^-	hydrogen carbonate ion or bicarbonate ion
		CO_3^{2-}	carbonate ion
		* CrO_4^{2-}	chromate ion
		* $Cr_2O_7^{2-}$	dichromate ion
		PO_4^{3-}	phosphate ion
		AsO_4^{3-}	arsenate ion

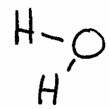
* additional ions that you come across

Formulas, Compounds & the Mole

Formula weight (FW): sum of masses of elements in the formula.

Example: H_2O water

H	$2 \times 1.0079 =$	2.0158
O	$1 \times 15.9994 =$	$\underline{15.9994}$
		18.0152



H_2O is made of nonmetals, so it is a covalent compound
The smallest part of H_2O that still has H_2O characteristics is the molecule.
$\therefore$ one tiny little molecule of H_2O "weighs" (has a mass of) 18.0152 amu
and FW = 18.0152 amu/molecule.

and if you have 1 mole ($N_A = 6.02 \times 10^{23}$ molecules) of H_2O,
it would "weigh" 18.0152 grams
The FW = 18.0152 g/mol of H_2O molecules.

since the density of water ~ 1.00 g/mL (depends on T)
you would have ~ 18 mL of H_2O.

Note: since water is a molecule, FW can also be molecular wt.

Example: How many molecules of H_2O are in 100. mL of H_2O?
Plan: $\text{mL } H_2O \xrightarrow[\text{use density}]{(1)} \text{g } H_2O \xrightarrow[MW]{(2)} \text{mol } H_2O \xrightarrow[N_A]{(3)} \text{molecules } H_2O$

we know
(1) $D(\text{g/mL}) = \dfrac{\#g}{\#mL} \quad \therefore \#g = D \times \#mL = 1.00\ \text{g/mL} \times 100.\ \text{mL} = 100.\ \text{g}$

(2) $MW(\text{g/mol}) = \dfrac{\#g}{\#mol} \quad \therefore \#mol = \dfrac{\#g}{MW} = \dfrac{100.\ g}{18.0\ g/mol} = 5.56\ \text{mol } H_2O$

(3) $N_A = \dfrac{\#\text{ particles}}{\#\text{ mol}} \quad \therefore \#\text{molecules} = N_A \times \#mol = 6.02 \times 10^{23}\ \dfrac{\text{molecules}}{\text{mol}} \times 5.56\ \text{mol}$
$= 3.35 \times 10^{24}$ molecules H_2O

OR

$$\#\text{molecules } H_2O = 100\ \text{mL } H_2O \times \overset{(1)}{\frac{1.00\ g}{1.00\ mL}} \times \overset{(2)}{\frac{1\ \text{mol } H_2O}{18.0\ g\ H_2O}} \times \frac{6.02 \times 10^{23}\ \text{molecules } H_2O}{1\ \text{mole } H_2O}$$

Example: Calculate formula weight of $Al_2(SO_4)_3 \cdot 18\, H_2O$

aluminum sulfate : $Al_2(SO_4)_3$ — anhydrous (no waters attached)

hydrated aluminum sulfate : $Al_2(SO_4)_3 \cdot 18\, H_2O$ — hydrate

	exact		inexact		
Al	2	×	26.98	=	53.96
S	3	×	32.06	=	96.18
O	$(\overset{30}{\overbrace{12 + 18}})$	×	16.00	=	480.0
H	36	×	1.008	=	36.29
					$666.4\cancel{3}$ g/mole formula weight

∴ if we have 1 mole of this compound, what do we really have ?

1 mole $Al_2(SO_4)_3 \cdot 18\, H_2O \equiv 6.022 \times 10^{23}$ formula units

(666.4 g) $\equiv$ 2 moles of Al (53.96 g)

$\equiv 2 \times 6.022 \times 10^{23}$ atoms of Al

$\equiv$ 3 moles of S (96.18 g)

$\equiv$ 30 moles of O

$\equiv$ 18 moles of H_2O ($18 \times 18.0 = 324$ g H_2O)

Percent Composition and Formulas of Compounds

percent composition : percent by mass of each element in the compound.

Example: Calculate the percent by mass of the elements in $Al_2(SO_4)_3 \cdot 18\, H_2O$

Assume: you have 1 mole of compound ≡ 666.4 g in this case (see above)

$$\% Al = \frac{\text{mass of Al in formula unit}}{\text{formula weight}} \times 100 = \frac{53.96}{666.4} \times 100 = 8.097\ \%$$

$$\% S = \frac{\text{mass of S in formula unit}}{\text{formula weight}} \times 100 = \frac{96.18}{666.4} \times 100 = 14.43\ \%$$

$$\% O = \frac{\text{mass of O}}{\text{F.W.}} \times 100 = \frac{480.0}{666.4} \times 100 = 72.03\ \%$$

$$\% H = \frac{\text{mass of H}}{\text{F.W.}} \times 100 = \frac{36.29}{666.4} \times 100 = 5.446\ \%$$

$100.00\cancel{3}$ %

All samples of hydrated aluminum sulfate have this composition.
(Law of Definite Proportions)

Law of Multiple Proportions: If two elements combine to form more than one compound, the ratio of the masses can be expressed in small whole numbers

e.g. H , O $\quad H_2O$ (water) $\quad H_2O_2$ (hydrogen peroxide) $\quad \therefore \dfrac{\text{mass of O in } H_2O}{\text{mass of O in } H_2O_2} = \dfrac{1}{2}$

Derivation of Formulas from Elemental Composition

Many times in the laboratory, a chemist will synthesize a compound. To help prove that she prepared what she thought she prepared, she will send a sample of the new compound to a commercial laboratory for elemental analysis. From this information, she can deduce the simplest or empirical formula (the smallest whole number ratio of atoms present in a compound).

Examples of simplest (empirical) formulas:

TRUE MOLECULAR FORMULA	SIMPLEST FORMULA
C_6H_6 (benzene)	CH
As_4O_{10}	As_2O_5
SO_2	SO_2

Example: Consider a compound that only contains carbon and hydrogen. The results come back: 85.6 % C and 14.4 % H. What is the simplest (empirical formula for the compound?

Step ①: Assume we have 100 g of compound - to make calculations easier.
$\therefore$ we have 85.6 g C and 14.4 g H.

Step ②: Recall that formulas involve ratios of atoms or moles of atoms <u>NOT</u> mass.
$\therefore$ we must change mass of element $\longrightarrow$ moles of element.

$$\# \text{ moles } C = \frac{85.6 \text{ g C}}{12.0 \text{ g/mol}} = 7.13 \text{ moles C} \qquad \text{since mol} = \frac{g}{AW}$$

$$\# \text{ moles } H = \frac{14.4 \text{ g H}}{1.00 \text{ g/mol}} = 14.4 \text{ moles H}$$

Recall that the elements in a formula are in a ratio of whole numbers to each othe

Step (3) Choose the smallest number of moles to use as a divisor for the other numbers.

$$\text{for C} \quad \frac{7.13}{7.13} = 1.00$$

$$\text{for H} \quad \frac{14.4}{7.13} = 2.02$$

But the ratios must be whole numbers.

$$\therefore \frac{\text{mol C}}{\text{mol H}} = \frac{1}{2}$$

$\therefore$ empirical formula for the compound is CH_2

To continue, the chemist knows from another experiment that the molecular weight of her compound is 42. What is the true or actual formula?

The simplest formula, CH_2, has as its formula weight

$$\begin{array}{llll} C: & 1 \times 12.011 & = & 12.011 \\ H: & 2 \times 1.008 & = & \underline{2.016} \\ & & & 14.027 \text{ amu} \end{array}$$

But,

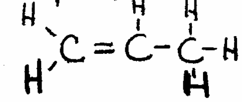
$$\text{actual formula weight} = \overset{\text{(simplest)}}{\text{empirical}} \text{ formula weight} \times \underline{\text{whole number}}$$

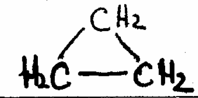
$$42 = 14x$$

$$x = 3$$

$\therefore$ actual formula $= (CH_2)_3 = C_3H_6$

So, sample could be propene or cyclopropane.





Example: What is the simplest formula for a compound: 65.20% As, 34.80% O ?

	(1) Assume 100 g		(2) change to moles	(3) divide by smallest #
As	65.20 g	$\rightarrow$	$\frac{65.20\,g}{74.92\,g/mol} = 0.8703$	$\frac{0.8703}{0.8703} = 1.000$
O	34.80 g	$\rightarrow$	$\frac{34.80\,g}{16.00\,g/mol} = 2.175$	$\frac{2.175}{0.8703} = 2.499$

Now, you have found the formula $As_1O_{2.499}$

What do you do to change subscripts to whole numbers?

You do <u>NOT</u> round off! to give either AsO_2 or AsO_3

You <u>DO</u> multiply thru by 2 to give As_2O_5.

Note: only round off when < 0.1 or so from whole number.

e.g. $FeO_{1.33}$ does not round off to FeO. Multiply by 3 to give Fe_3O_4.

Additional Problem:

How many atoms of Oxygen are contained in a 9.80g sample of H_2SO_4? (MW H_2SO_4 = 98.0 g/mol)

Plan: g $H_2SO_4 \xrightarrow{(1)}$ moles $H_2SO_4 \xrightarrow[\text{either}]{(2)}$ moles O $\xrightarrow{(3)}$ atoms O

$\xrightarrow{\text{or}}$ molecules $H_2SO_4 \rightarrow$ atoms O

(1) moles $H_2SO_4 = \frac{9.80g}{98.0\,g/mol} = 0.100$ moles H_2SO_4

(2) moles O $= 4 \times$ moles $H_2SO_4 = 0.400$ moles O since $\frac{4 \text{ moles O}}{1 \text{ mol } H_2SO_4}$

(3) atoms O $= 6.02 \times 10^{23} \frac{\text{atoms}}{\text{mole}} \times 0.400$ moles $= \underline{2.41 \times 10^{23} \text{ atoms O}}$

#57. If Epsom salt, $MgSO_4 \cdot x\,H_2O$ is heated to 250°C, all the water of hydration is lost. On heating 1.687 g sample of the hydrate, 0.824 g of $MgSO_4$ remains. How many molecules of water occur per formula unit of $MgSO_4$ in epsom salt?

Try to write an equation!

$$\underset{1.687\,g}{MgSO_4 \cdot x\,H_2O} \xrightarrow{\Delta} \underset{0.824\,g}{MgSO_4} + \underset{?\,g}{x\,H_2O}$$

Δ: represents a tiny bunsen burner

x = moles of water per 1 mol of epsom salt

Law of conservation of matter says that in any ordinary process or reaction (not a nuclear reaction),

mass of reactants = mass of products

You can easily see that the mass of water in the epsom salt sample must be $1.687 - 0.824 = 0.863\,g\ H_2O$

Since formulas deal with ratios of moles, not grams, we must convert!

$$\#\text{moles } MgSO_4 = \frac{0.824\,g}{120.4\,g/mol} = 0.00684\ mol$$

$$\#\text{moles } H_2O = \frac{0.860\,g}{18.0\,g/mol} = 0.0478\ mol$$

if we divide, we know how many moles of H_2O per mole of $MgSO_4$ which is the same ratio as the number of molecules of H_2O per formula unit of $MgSO_4$.

$$\frac{\#\text{ moles of } H_2O}{\#\text{ moles } MgSO_4} = \frac{0.0478\ mol\ H_2O}{0.00684\ mol\ MgSO_4} = 6.99 \text{ or } 7$$

since it must be a whole number

∴ formula of epsom salt must be: $MgSO_4 \cdot 7H_2O$