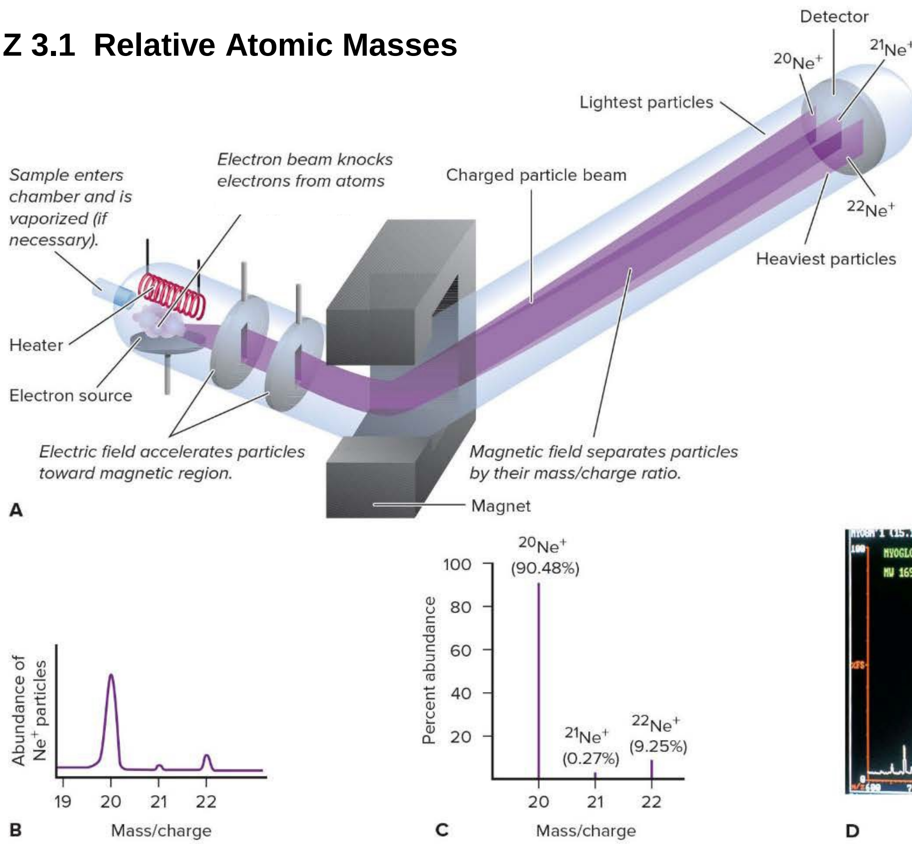
STOICHIOMETRY

Z Ch 3; H Ch 1-4, 22-1

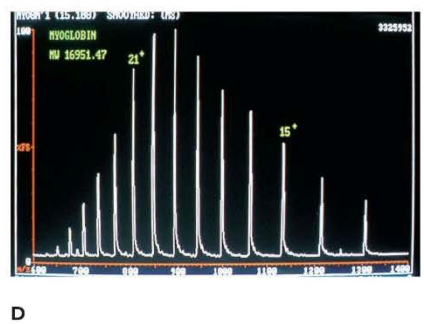
"Stoichiometry is the science of measuring the quantitative proportions or mass ratios in which chemical elements stand to one another." **Jeremias Benjamin Richter, 1792**

Richter introduced the word stoichiometry (Greek, *stoicheion* - element and *metron*-measure)

Z 3.1 Relative Atomic Masses



Horse myoglobin – common molecular weight calibrant for mass spectrometers



Mass spectral data of naturally occurring neon, composed of three isotopes.

EX 1. From the following data and your periodic table determine the percent natural abundance of the following two isotopes:

isotope	mass
boron-10	10.01294
boron-11	11.00931

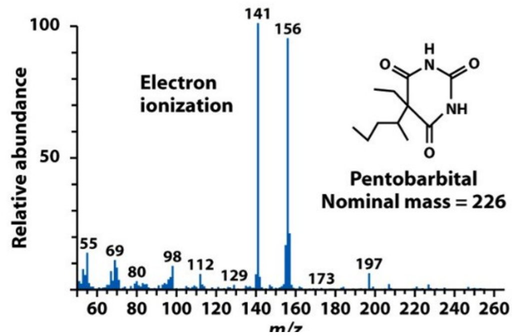
EX 2. Copper has two isotopes. 30.91% of the mass of copper is due to ^{65}Cu whose isotopic mass is 64.9278. Calculate the mass of the other isotope and give its complete symbol.

H 22-1, Box 22-4 Mass Spectrometry

Mass spectrometry developed quickly after Thomson had demonstrated that relative atomic and molecular masses could be measured directly by observing the deflections of ions in electric and magnetic fields. With the advent of commercial instrumentation in the 1950s, mass spectrometry became routinely used for not only accurate molecular mass determination but also for yielding valuable information about chemical formulas and molecular structure such as unraveling the sequence of amino acids in proteins.

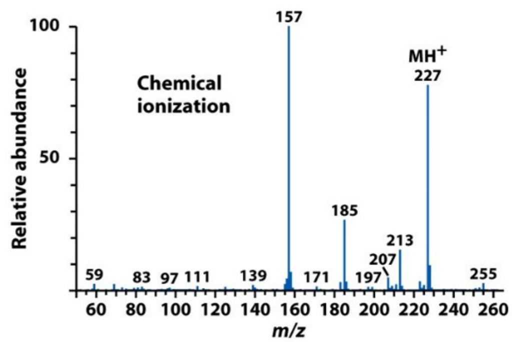
Electron Impact Ionization (EI)

A sample is bombarded by 70 eV electrons which are well in excess of the energy required to ionize any molecule with the excess kinetic energy causing the ions to highly fragment where often the molecular ion cannot be discerned. Fragmentation patterns are characteristic of the molecular structure as seen on the right.



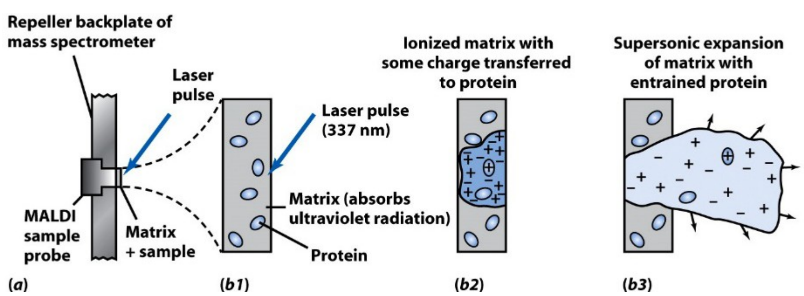
Chemical Ionization (CI)

A soft ionization technique (imparts little excess kinetic energy in the molecule and less fragmentation) where the sample is mixed with a reagent gas. Upon ionization of this gas ions are produced which transfer a proton to the sample producing MH^+ ions. Less fragmentation is found in the resulting mass spectrum seen on the right (same molecule as in EI spectrum above).

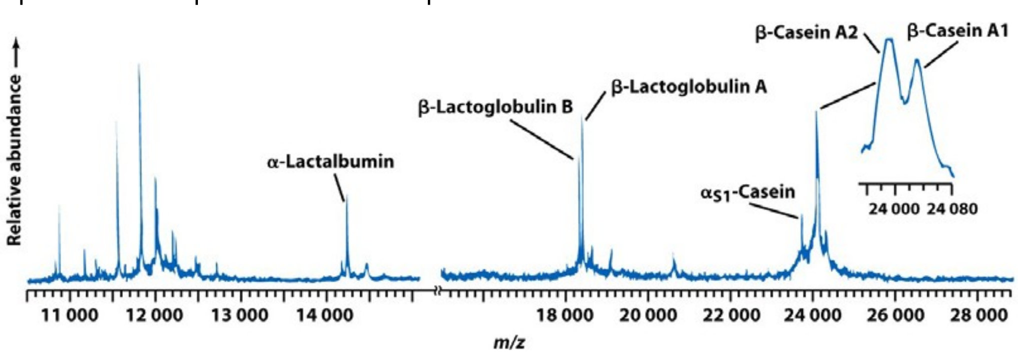


Matrix-Assisted Laser Desorption Ionization (MALDI)

Another soft ionization technique where the sample is dissolved in a UV-absorbing compound, evaporated to leave a crystalline matrix containing M, and then the matrix is vaporized with a UV laser pulse. This evaporation expands the matrix into the gas phase along with the charged analyte.



The technique allows samples whose *m*/*z* is up to ~ 10^6.



Z 3.2 Atoms and the Mole

relative atomic mass (RAM) => actual mass of one atom (Lorenzo Romano Amadeo Carlo **Avogadro,** Conte di Quarequa e di Cereto)

Avogado's Number defined to be the number of atoms in exactly 12 g of ^{12}C (1 mole)

$$No = 6.02214 \times 10^{23}\ mol^{-1}$$

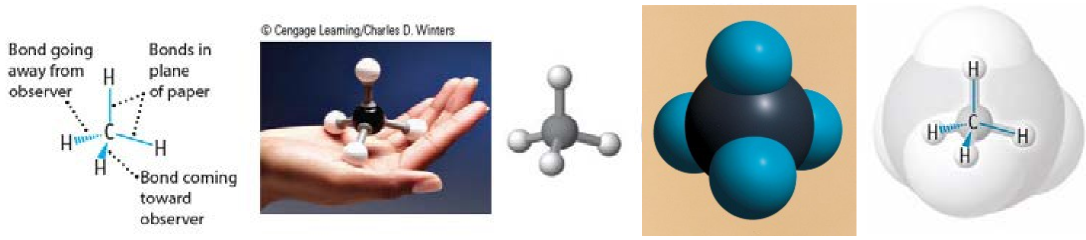
EX 3. What is the mass of a single carbon-12 atom?

EX 4. A single atom of an element has a mass of 2.10730×10^{-22} g. What is the element assuming that it has only one isotope?

EX 5. How many atoms of Fe are in 8.232 g Fe?

EX 6. Lithium has a density of 0.534 g cm^{-3}. Determine the volume per atom in lithium.

COMPOSITION OF COMPOUNDS



Simple perspective drawing | Plastic model | Ball-and-stick model | Space-filling model | The three representations in a single drawing.

Z 3.3 Molar Mass: atoms <=> mole <=> mass

EX 7. For exactly 2 kg methane, CH_4 [H = 1.0079, C = 12.011; M_{CH_4} = 4(1.0079) + 12.011) = 16.0426]

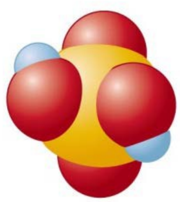
a) How many moles of methane does it contain?

b) How many grams of hydrogen does it contain?

c) How many atoms of hydrogen does it contain?

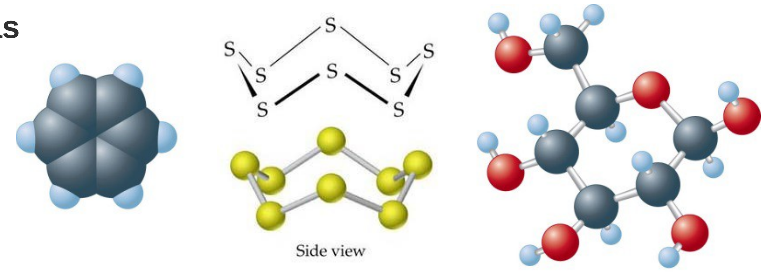
Z 3.5, 3.11 Percent Composition by Mass

EX 8. Find the percent composition of sulfuric acid, H_2SO_4 ; [H = 1.0079, S = 32.065, O = 15.999; $M_{H_2SO_4}$ = 2(1.0079) + 32.065 + 4(15.999) = 98.0768]



Z 3.6 Determining the Formula of a Compound

empirical and **molecular formulas**



$C_6H_6 = (CH)_6$ $S_8 = (S)_8$ $C_6H_{12}O_6 = (CH_2O)_6$

from mass data:

EX 9. Find the empirical formula of an iron oxide if 1.596 g of the oxide contains 1.116 g of iron. [Fe= 55.845, O = 15.999]

from percent composition:

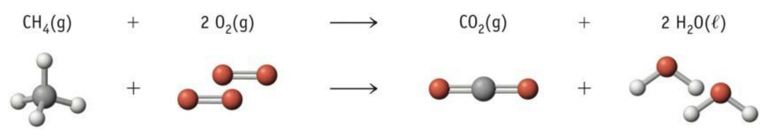
EX 10. A compound of sulfur and fluorine contains 25.2% S. [S = 32.065, F = 18.998]

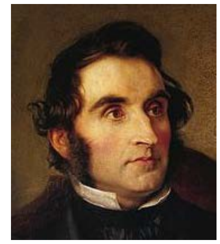
a) What is its empirical formula?

b) If 0.0450 moles have a mass of 11.4 g what is its molecular formula?

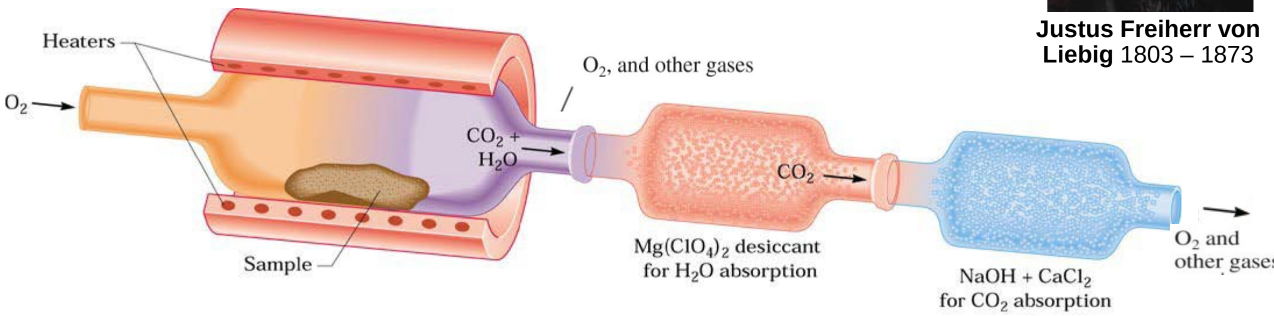
from chemical analysis

combustion





Justus Freiherr von Liebig 1803 – 1873



Combustion train for measuring the amounts of carbon and hydrogen in a compound.

EX 11. An unknown compound contains only C, H, N, and O. Burning 1.261 g of the compound in excess oxygen produced 2.286 g of CO_2 and 0.5805 g of water vapor. 0.364 g of nitrogen gas were also collected. What is the empirical formula of the unknown? [C = 12.011, H = 1.0079, N = 14.0067, O = 15.999; M_{CO_2} = 44.009; M_{H_2O} = 18.0148]

CHEMICAL EQUATIONS

"Nothing is created ... and it may be considered as a general principle that in every operation [reaction] there exists an equal quantity of matter before and after the operation ... It is on this principle that is founded all the art of performing chemical experiments ..." **Antoine Laurent de Lavoisier, 1785**

Lavosier's Law of Conservation of Mass - in a chemical reaction matter is neither created nor destroyed:

Z 3.7, 3.8 Chemical Equations / Balancing

indicate the **physical state**

$HCl(aq) + NaHCO_3(s)$ =>
$NaCl(aq) + CO_2(g) + H_2O(l)$

(*g*)	The substance is in the gaseous state or vapor state.
(ℓ)	The substance is in the liquid state.
(*fl*)	The substance is in a fluid state (either gas or liquid).
(*s*)	The substance is in the solid state.
(*cr*)	The substance is crystalline.
(*aq*)	The substance is dissolved in water (in aqueous solution)
(*sln*)	The substance is in solution.

conservation of mass => **balance** equations

1. by inspection

______$NaBr$ + ______H_3PO_4 → ______HBr + ______Na_3PO_4

2. most complicated first

______$C_3H_5N_3O_9$ → ______CO_2 + ______N_2 + ______H_2O + ______O_2

3. algebraic method

______HNO_2 + ______HI → ______NO + ______I_2 + ______H_2O

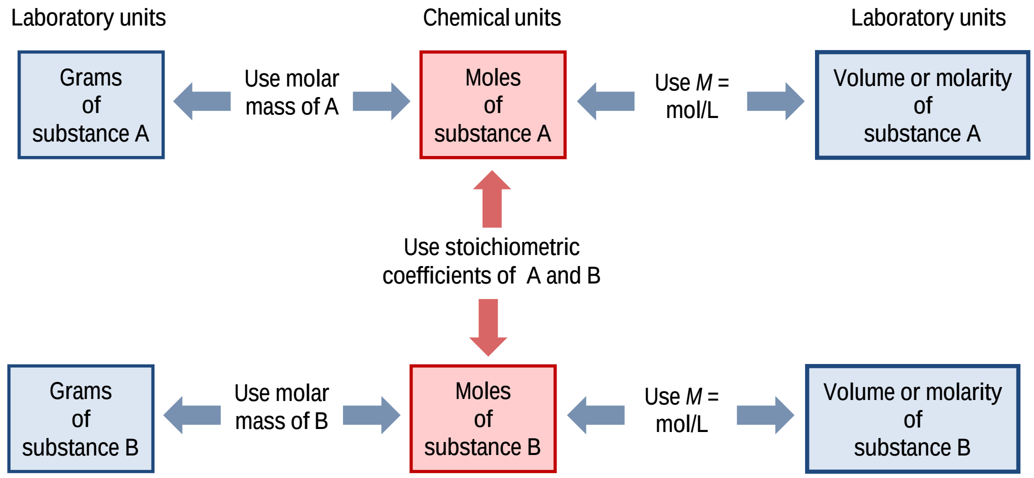
Z 3.9 **Stoichiometry** - the mass relationship between reactants and products

$$2\ C_5H_{10}(l) + 15\ O_2(g) \rightarrow 10\ CO_2(g) + 10\ H_2O(l)$$

LOTS OF INFORMATION

2 C_5H_{10} molecules + 15 O_2 molecules → 10 CO_2 molecules + 10 H_2O molecules
4 C_5H_{10} molecules + 30 O_2 molecules → 20 CO_2 molecules + 20 H_2O molecules
2 N_O C_5H_{10} molecules + 15 N_O O_2 molecules → 10 N_O CO_2 molecules + 10 N_O H_2O molecules
2 mol C_5H_{10} + 15 mol O_2 → 10 mol CO_2 + 10 mol H_2O
140.268 g C_5H_{10} + 479.97 g O_2 → 440.09 g CO_2 + 180.148 g H_2O
620.24 g → 620.24 g

Solving Stoichiometry Equations



EX 12. For the above reaction [H = 1.0079, C = 12.011 => M = 70.134]

a) How many grams of oxygen are necessary to completely oxidize 37.00 g of C_5H_{10}?

b) How many grams of carbon dioxide are formed?

c) How many grams of water are formed?

d) If in another reaction 1.25 L of O_2 were consumed, how many liters of CO_2 were produced? Assume *T, P* same before and after the reaction. (Gay-Lussac 's Law of Combining Volumes)

H 1-4; Z 3.9 Stoichiometric Calculations: Limiting Reactants

limiting reactant – reactant present in limited supply that determines the amount of product produced

EX 13. A mixture containing 20.0 g of methane (CH_4) and 100. g of oxygen is ignited and burned. What substances will be found in the mixture after the reaction stops?
[C = 12.011, H = 1.0079 => M_{CH_4} = 12.011 + 4(1.0079) = 16.0426; O = 15.999 => M_{O_2}= 2(15.999) = 31.998; M_{CO_2}= 12.011 + 2(15.999) = 44.009]

EX 14. When hydrogen sulfide gas is bubbled into a solution of sodium hydroxide, sodium sulfide and water are produced. How many grams of sodium sulfide are formed if 2.50 g of hydrogen sulfide is bubbled into a solution containing 1.85 g of sodium hydroxide?
[Na = 22.990, O = 15.999, H = 1.0079 => M_{NaOH} = 39.9969; S = 32.065 => M_{H2S} = 32.065 + 2(1.0079) = 34. 0808; M_{Na2S} = 78.045]

Z 3.10 Calculations Involving a Limiting Reactant: Yields

yields

theoretical yield - yield (mass of product) predicted from stoichiometry assuming reaction goes to completion without loss or side reactions => maximum amount of product possible

actual yield - yield (mass of product) actually obtained experimentally

percent yield = 100 × (actual yield / theoretical yield)

EX 15. Determine the % yield if 3.12 g of CH_4N_2O is isolated when 5.11 g of NH_3 and excess CO_2 react according to:

$$2\ NH_3 + CO_2 \rightarrow CH_4N_2O + H_2O$$

[M_{NH3} = 17.0307; M_{CH4N2O} = 60.0556 g/mol]