Chemistry 3A

Introductory General Chemistry

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- The Mole: Avogadro’s Number
- Moles and Atoms: Conversions
- Molar Mass
- Moles and Mass: Conversions
- Mass and Particle Number
- Percent Composition
- Empirical Formulas
- Percent of Water in a Hydrate
- Molecular Formulas

Avogadro's Number

- Counting atoms and molecules and submicroscopic particles one-by-one is impossible task
- Italian scientist Amadeo Avogadro devised the **mole**
- **Avogadro's Number** is the number of representative particles of a substance equal to **6.022×10^{23}**
- SI unit for amount of a substance
- The official symbol for Avogadro's Number is N_A

Avogadro's Number

- The number is of a count of particles making up 1 mole (1 mol)

Your online book includes YouTube link on mole concept

Oh, a mole is a name of a mammal too

Substance	**Representative Particle**
Most elements, particularly metals	Atom
Diatomic elements: (H_2, O_2, N_2, F_2, Cl_2, Br_2, I_2) Many molecular compounds: H_2O, CO_2	Molecule
Ionic Compounds: NaCl, $Ca(NO_3)_2$	Formula Unit

Moles to/from Atoms/Molecules/Particles

Fun with conversions

1 mole = 6.022×10^{23} particles/atoms/molecules

Official abbreviation for mole is **mol**

How many moles in 4.72×10^{24} atoms C?

$$4.72 \times 10^{24} \cancel{\text{atoms C}} \times \frac{1\ \text{mol C}}{6.022 \times 10^{23} \cancel{\text{atoms C}}} = 7.84\ \text{mol C}$$

Avogadro's Number is a defined CONSTANT, not a measured quantity. It is precise to $6.02214076 \times 10^{23}$

Step 3: Think about your result. **BOOK MISTAKE**

The given number of carbon atoms was greater than Avogadro's number, so the number of moles of C atoms is greater than 1 mole. Since Avogadro's number is a measured quantity with three significant figures, the result of the calculation is rounded to three significant figures.

Moles to/from Atoms/Molecules/Particles

How many atoms of H (hydrogen) are in 1 mol H_2O?

$$1\ \cancel{\text{mol H}_2\text{O}} \times \frac{6.022 \times 10^{23}\ \cancel{\text{molecules H}_2\text{O}}}{1\ \cancel{\text{mol H}_2\text{O}}} \times \frac{2\ \text{atoms H}}{1\ \cancel{\text{molecule H}_2\text{O}}}$$

$$= 6.022 \times 10^{23}\ \text{atoms H}$$

One conversion factor makes use of Avogadro's number. The 2nd relates to how many atoms are in a particular molecule

Another Conversion Example

An amount of sulfuric acid (H_2SO_4) containing 4.89×10^{25} oxygen (O) atoms is obtained. How many moles sulfuric acid are there?

$$4.89 \times 10^{25}\ \cancel{\text{atoms O}} \times \frac{1\ \cancel{\text{molecule H}_2\text{SO}_4}}{4\ \cancel{\text{atoms O}}} \times \frac{1\ \text{mol H}_2\text{SO}_4}{6.022 \times 10^{23}\ \text{molecules H}_2\text{SO}_4}$$

$$= 20.3\ \text{mol H}_2\text{SO}_4$$

Like the previous problem, Avogadro’s number was used along with look at one atom that is part of a molecule.

Molar Mass

- The term **molar mass** refers the mass (in grams) of one mole of a substance.
- The units are (usually) grams per mole

Whenever the term mass is used, it will refer to a quantity whose units will be in grams (or a power of 10 in grams: kilograms [kg], milligrams [mg], micrograms [μg], etc). A molar mass will be grams per mole.

- The substance can be atoms (pure element), molecules, or particles

Note the old terms atomic weight (for pure elements and molecular weight for molecules and compounds are deprecated

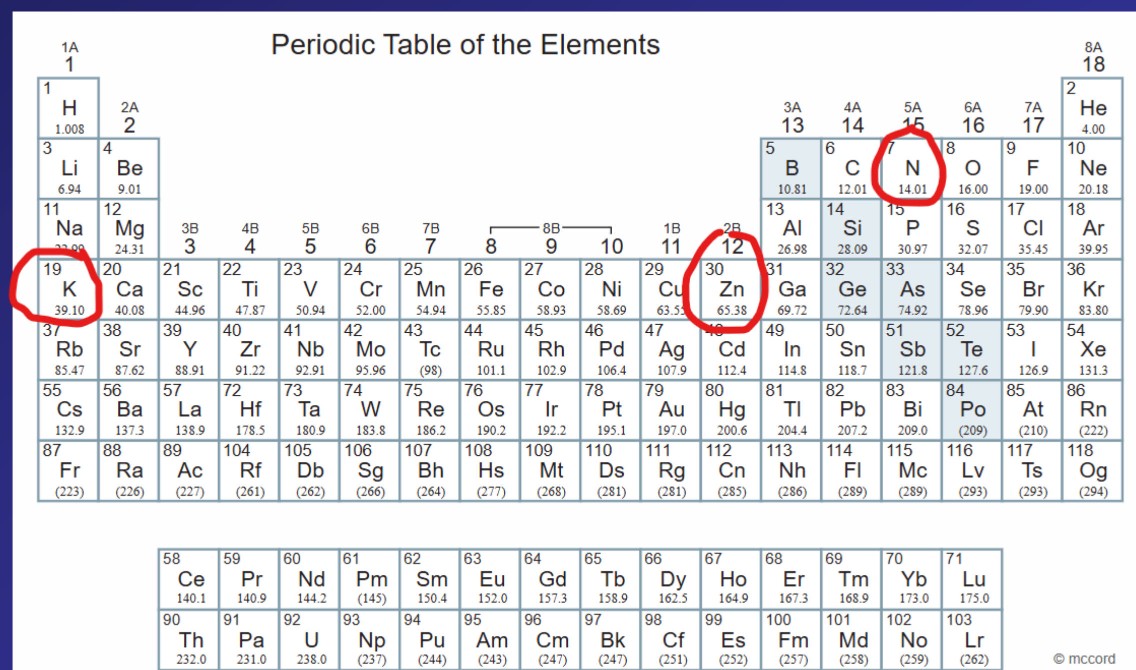
Determining Molar Mass

For atoms of the pure elements, the molar mass is on the Periodic Table

Nitrogen (N): 14.01 grams per mole (g/mol)

Zinc (Zn): 65.38 g/mol

Potassium (K): 39.10 g/mol



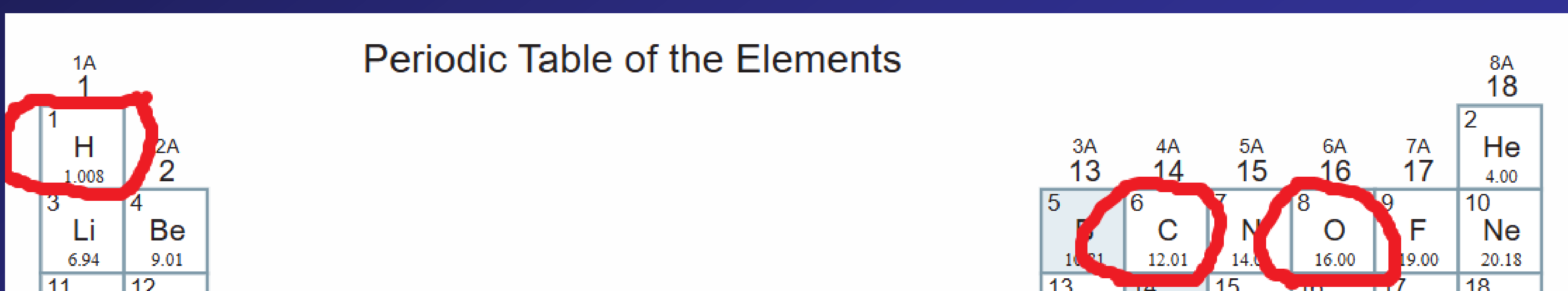
Determining Molar Mass

For compounds/molecules the total mass is computed (by addition) of the component elements taken from the Periodic Table:

H_2O (water): $\left(\frac{2\text{ mol H}}{1\text{ mol H}_2\text{O}} \times \frac{1.008\text{ g H}}{1\text{ mol H}}\right) + \left(\frac{1\text{ mol O}}{1\text{ mol H}_2\text{O}} \times \frac{16.00\text{ g O}}{1\text{ mol O}}\right) =$ $\mathbf{18.016\ g/mol}$

CO_2 (carbon dioxide):

$$\left(\frac{1\text{ mol C}}{1\text{ mol CO}_2} \times \frac{12.01\text{ g C}}{1\text{ mol C}}\right) + \left(\frac{2\text{ mol O}}{1\text{ mol CO}_2} \times \frac{16.00\text{ g O}}{1\text{ mol O}}\right) = \mathbf{44.01\ g/mol}$$

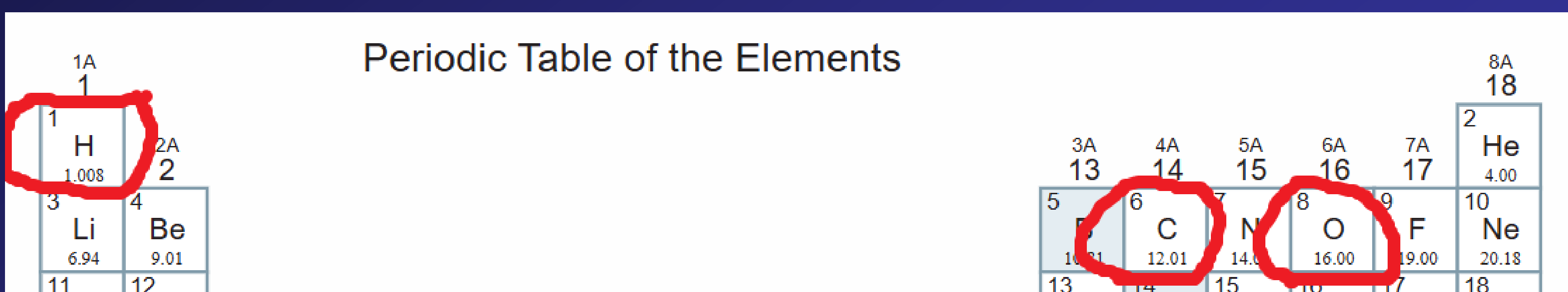


Computing Molar Mass

You don’t really have to set up the expression the way it was shown. The other way is the long form to show how all units:

H_2O: $$2 \times 1.008\frac{\mathrm{g}}{\mathrm{mol}}\mathrm{H} + 16.00\frac{\mathrm{g}}{\mathrm{mol}}\mathrm{O} = 18.016\frac{\mathrm{g}}{\mathrm{mol}}\mathrm{H_2O}$$

CO_2: $$12.01\frac{\mathrm{g}}{\mathrm{mol}}\mathrm{C} + 2 \times 16.00\frac{\mathrm{g}}{\mathrm{mol}}\mathrm{O} = 44.01\frac{\mathrm{g}}{\mathrm{mol}}\mathrm{CO_2}$$



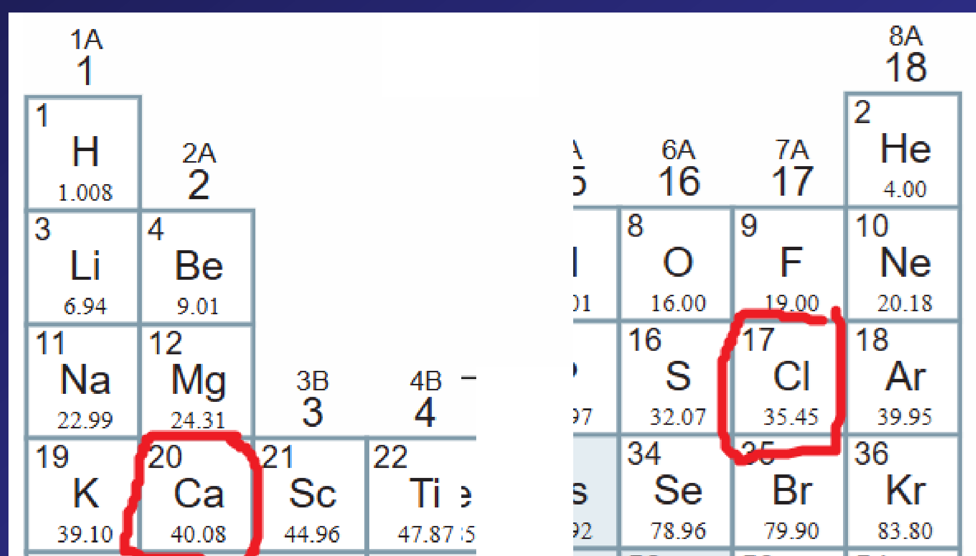
Moles ↔ Mass

Learning by example

- 3.00 mol calcium chloride ($CaCl_2$) is needed for experiment
- Its computed molar mass =

$$\left(1 \times \frac{40.08\ \mathrm{g}}{\mathrm{mol}}\mathrm{Ca}\right) + \left(2 \times \frac{35.45\ \mathrm{g}}{\mathrm{mol}}\mathrm{Cl}\right) = \frac{110.98\ \mathrm{g}}{\mathrm{mol}}\mathrm{CaCl_2}$$

Needed amount: $3\ \mathrm{mol\ CaCl_2} \times \frac{110.98\ \mathrm{g}}{\mathrm{mol}}\mathrm{CaCl_2} = 333\ \mathrm{g\ CaCl_2}$



Moles ↔ Mass

Your book correctly points out that converting from particle counts to the observable mass of these particles will involve a two-step conversion

But this is not routine in chemistry or for chemists. It will only be an exercise to demonstrate you understand the concept

How many molecules in 20.0 g chlorine (Cl_2) gas?

$$20.0\ \mathrm{g\ Cl_2} \times \frac{1\ \mathrm{mol\ Cl_2}}{70.90\ \mathrm{g\ Cl_2}} \times \frac{6.022 \times 10^{23}\ \mathrm{molecules\ Cl_2}}{1\ \mathrm{mol\ Cl_2}}$$
$$= 1.70 \times 10^{23}\ \mathrm{molecules\ Cl_2}$$

Figure 5.5.1: Conversion from number of particles to mass, or from mass to number of particles requires two steps.

Percent Composition

- The **percent composition** is the percent by mass of each element in a compound

$$\%\text{ by mass} = \frac{\text{mass of element}}{\text{mass of compound}} \times 100\%$$

A compound has zinc & oxygen. A 20.00 g sample is decomposed, and found to have 16.07 g Zn. What is the percent composition of compound?

$$\%\text{Zn} = \frac{16.07\text{ g Zn}}{20.00\text{ g sample}} \times 100\% = 80.35\%\text{ Zn}$$

$$\%\text{O} = \frac{20.00\text{ g sample } - 16.07\text{ g O}}{20.00\text{ g sample}} \times 100\% = 19.65\%\text{ O}$$

% Composition from Formula

Dichlorine heptoxide (Cl_2O_7) is a very reactive compound used in organic synthesis

What is the percent composition of Cl_2O_7?

$$\%\mathrm{Cl} = \frac{2\ \mathrm{mol}\ \mathrm{C}l \times \dfrac{35.45\ \mathrm{g\ Cl}}{1\ \mathrm{mol\ Cl}}}{\left(2\ \mathrm{mol\ Cl} \times \dfrac{35.45\ \mathrm{g\ Cl}}{1\ \mathrm{mol\ Cl}} + 7\ \mathrm{mol\ O} \times \dfrac{16.00\ \mathrm{g\ O}}{1\ \mathrm{mol\ O}}\right)} \times 100\% = 38.76\%\ \mathrm{Cl}$$

$$\%\mathrm{O} = \frac{7\ \mathrm{mol\ Cl} \times \dfrac{16.00\ \mathrm{g\ O}}{1\ \mathrm{mol\ O}}}{\left(2\ \mathrm{mol\ Cl} \times \dfrac{35.45\ \mathrm{g\ Cl}}{1\ \mathrm{mol\ Cl}} + 7\ \mathrm{mol\ O} \times \dfrac{16.00\ \mathrm{g\ O}}{1\ \mathrm{mol\ O}}\right)} \times 100\% = 61.24\%\ \mathrm{O}$$

Since oxygen was the only element of two, it's also possible to take 100% - 38.76% = 61.24% to get the value

A Formula for Mass of Elements

To get the mass in grams of each element, suppose there are x of the compound Cl_2O_7 in a sample.

To calculate the grams of element Cl and of element O in Cl_2O_7, just use the formulas:

$$\text{mass of sample (g)} \times 38.76\%\ \text{Cl} = \text{mass of Cl (g)}$$
$$\text{mass of sample (g)} \times 61.24\%\ \text{O} = \text{mass of O (g)}$$

Example: a 12.50 g Cl_2O_7 sample has 4.845 g Cl and 7.655 g O

Empirical Formula Determination

- Recall that the definition of empirical formula is the lowest integer ratio of the elements in a compound. For instance, glucose has a molecular formula of $C_6H_{12}O_6$, but its empirical formula is CH_2O
- The reason for the empirical formula was because in analyzing a substance, it was the proportions of the elements chemists first saw in the analysis. They did not immediately have an understanding of how many atoms of each element actually made up a molecule or formula unit
- The process of getting the empirical formula is called elemental analysis

Elemental Analysis

1. Get exactly 100 g of the compound: enables the grams of a component element to also be the percentage of the component element
2. Determine from the mass in grams of a component element to moles of it using molar mass
3. Find the component element with the fewest (smallest number) moles of the compound, and use that number to divide the mole values of all other elements; the element with fewest moles should be 1
4. Step 3 should hopefully produce (almost) integer values in all other elements: those integers become the subscripts of the elements in the formula
5. In some cases, step 3 may be produce integer values: multiply each of moles by smallest whole number to convert each into whole number. Write formula

Elemental Analysis: Example

A compound is composed of 69.94% iron (Fe) and 30.06% oxygen (O). What is the empirical formula?

1. A 100 g sample should b 69.94 g Fe and 30.06 g O
2. Convert to moles each element

$$69.94 \text{ g Fe} \times \frac{1 \text{ mol Fe}}{55.85 \text{ g Fe}} = 1.252 \text{ mol Fe}$$

$$30.06 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 1.879 \text{ mol O}$$

3. Divide all values by the smallest (mole) value:

$$\frac{1.252 \text{ mol Fe}}{1.252} = 1 \text{ mol Fe} \qquad \frac{1..879 \text{ mol O}}{1.252} = 1.501 \text{ mol O}$$

4. Try to make all values a whole number. Multiplying by 2 will achieve this:

$$1 \text{ mol Fe} \times 2 = 2 \text{ mol Fe} \qquad 1.501 \text{ mol O} \times 2 = 3 \text{ mol O}$$

Formula: Fe_2O_3

Bluish-Green vs White Copper Sulfate

- Copper(II) sulfate is a typical ionic compound which is white in color as a solid
- But when hydrated, H_2O molecules coordinate around the copper atom through the orbitals of its *d* electrons, and this coordinate bonding creates a bluish-green color for the compound

copper(II) sulfate pentahydrate ($CuSO_4 * 5\ H_2O$)

- Water molecules actually coordinate with formula units of many ionic compounds. Metal atoms in anhydrous form are often colored, but this bonding to H_2O molecules can cause a different color

Other Hydrates: Cobalt(II) Chloride

- Useful to know the percent water in a hydrate

What is the % hydrate of cobalt(II) chloride hexahydrate ($CoCl_2 \bullet 6\ H_2O$)?

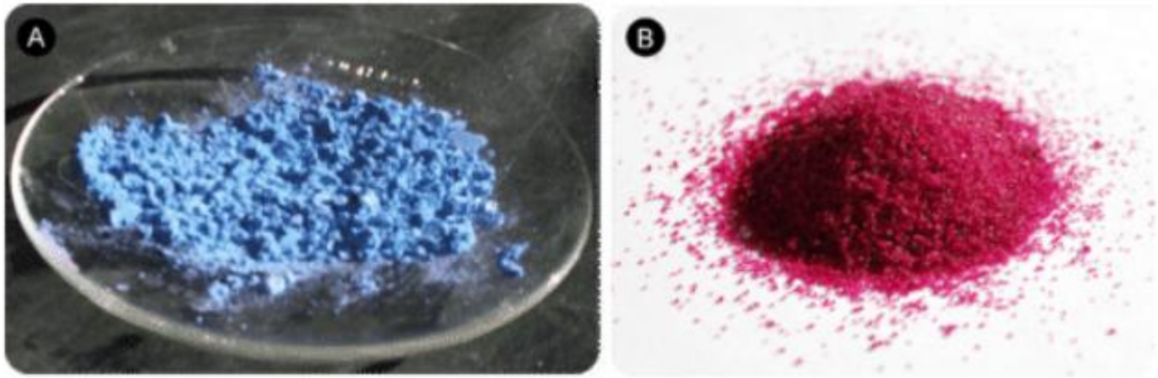


Figure 5.8.2: On the left is anhydrous cobalt (II) chloride, $CoCl_2$. On the right is the hydrated form of the compound called cobalt (II) chloride hexahydrate, $CoCl_2 \cdot 6H_2O$. (Credit: (A) Martin Walker (Wikimedia: Walkerma); (B) Ben Mills

Percent Water in $CoCl_2 \cdot 6\ H_2O$

- Molar mass of H_2O known

18.02 g/mol

- Number of H_2O in the compound known, so mass of water molecules known

$$6\ \text{mol}\ H_2O \times \frac{18.02\ \text{g}}{\text{mol}} H_2O = 108.12\ \text{g}\ H_2O$$

- $CoCl_2 \cdot 6\ H_2O$ molar mass easily determined

$$58.93\ (\text{Co}) + 2 \times 35.45\ (\text{Cl}) + 108.12\ (6\ H_2O) = 237.95\ \text{g/mol}$$

- % mass of water:

$$\frac{108.12\ \text{g}\ H_2O}{237.95\ \text{g}} \times 100\% = 45.44\%\ H_2O$$

- Almost half the mass is water

Glucose and Sucrose

- Glucose is a monosaccharide (carbohydrate) essential to life, metabolized ("burned") using oxygen (O_2) to carbon dioxide (CO_2) and water (H_2O)
- Sucrose (table sugar) is a disaccharide of glucose and fructose,
  and fructose is an isomer of glucose easily converted to glucose in metabolism
- How does one distinguish between glucose and sucrose?

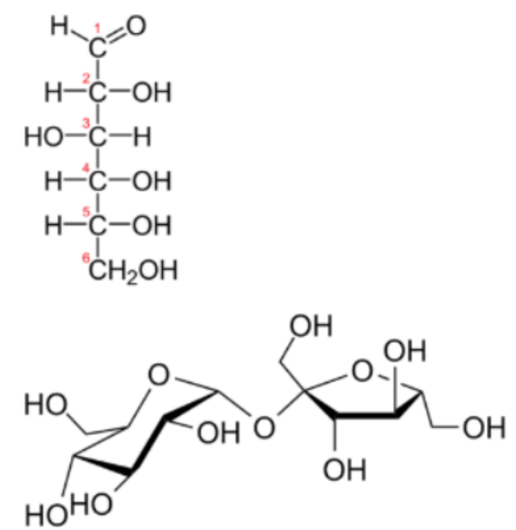
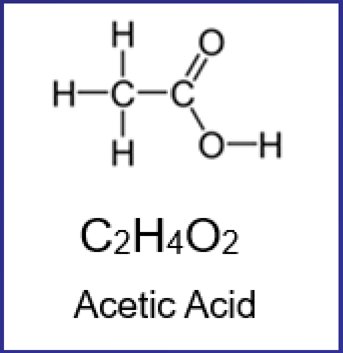
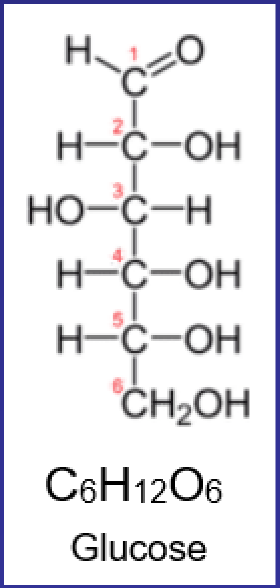


Figure 5.9.1: On top, the molecular structure of glucose. Below, the molecular structure of sucrose. please note: you do not need to understand the meaning of these structures at this point in the course.

Molecular Formula Determination

- Molecular formulas: the info about the *kind* and the *number* of atoms of each element present in a molecular compound
- The molecular formula and empirical formula can be identical in many cases, e.g. in methane (CH_4)
- Acetic acid (main acid in vinegar) and glucose have different molecular formulas but the same empirical formula: **CH_2O**
- Empirical formulas are learned from percent composition elemental analysis
- Molecular formulas require knowing molar mass of compound





Empirical → Molecular Formula

1. Calculate empirical formula mass (EFM): this is molar mass of empirical formula

2. Determine

$$\text{compound molar mass}/_{\text{EFM}} = \text{whole number or close to it}$$

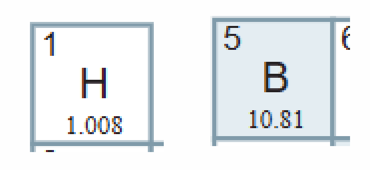
3. Multiply subscripts in empirical formula by whole number from Step 2 → this is molecular formula

Empirical → Molecular Formula

Let's apply the process to an example

Empirical formula of compound containing boron and hydrogen is BH_3 which has molar mass of 27.7 g/mol

1. EFM = 10.81 + 3×1.008 = 13.84 g/mol



2. $\frac{\text{molar mass}}{\text{EFM}} = \frac{27.7}{13.84} = 2$

3. $BH_3 \times 2 = B_2H_6$ ← molecular formula

Converting Mass/Moles/Gas Volume

- The online book's Mole Road Map
- Interrelates particle count, mass (in grams), and volume of a gas

Latter won't be important until we get to gases

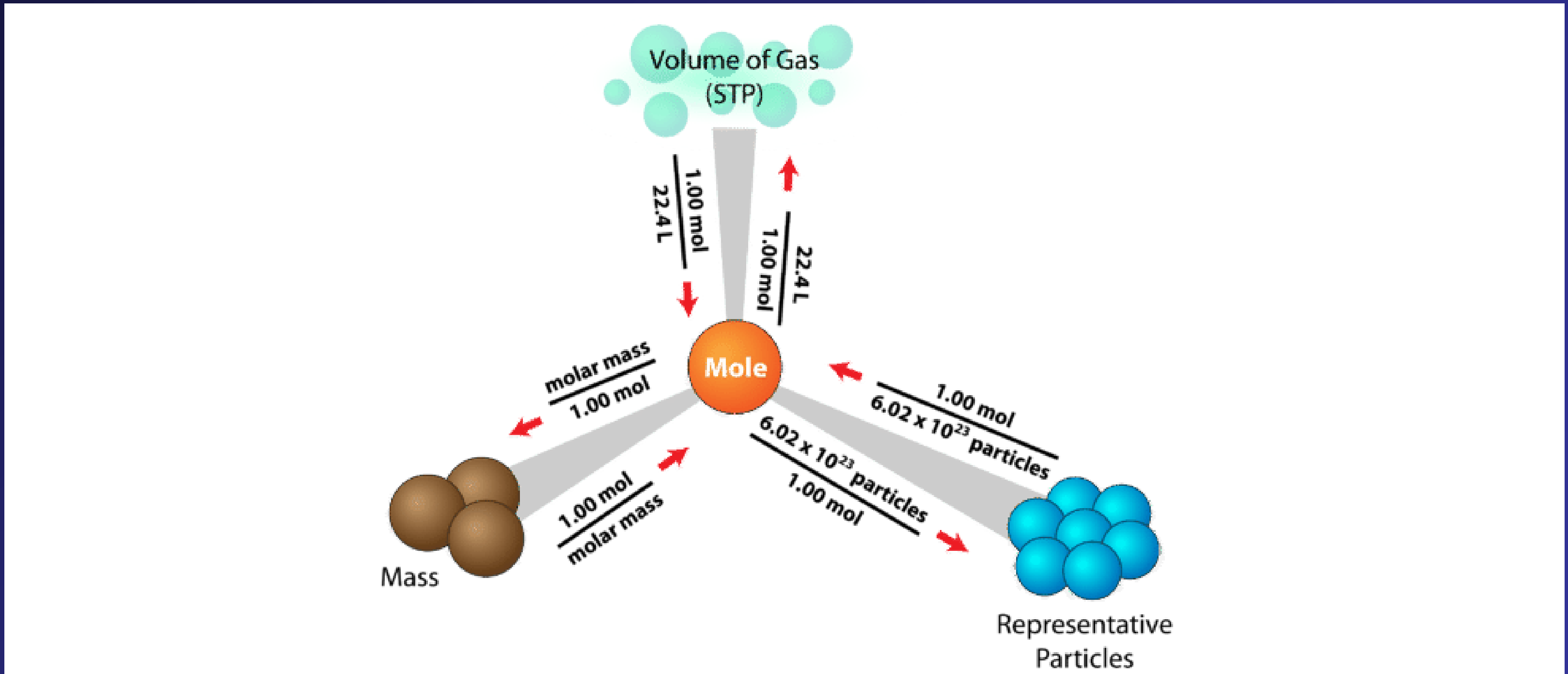


Figure 5.10.1: The mole road map shows the conversion factors needed to interconvert mass, number of particles, and volume of a gas.