Stoichiometry

– Studies the quantitative aspects of chemical reactions

3.1 The Mole

- Unit for amount of substance in terms of the number of entities (atoms, molecules, ...) in it.

1 mol of entities → # of atoms in 12 g of ^{12}C

1 atom of ^{12}C → 1.99265×10^{-23} g^{12}C (mass spectrometry)

12 g^{12}C×[1 atom/1.99265×10^{-23} g^{12}C] = 6.022×10^{23} atoms

⇒1 mol of entities → 6.022×10^{23} entities

- Avogadro's number (N_A) – number of entities per 1 mol → N_A = **6.022×10^{23} /mol**

- Conversion between moles and entities

[1 mol entities/6.022×10^{23} entities]

Example:

1) How many molecules of water are present in 2.7 mol of water?

2) How many atoms of hydrogen are present in 2.7 mol of water?

$$2.7\text{ mol }H_2O\left(\frac{6.022\times10^{23}\text{ molec. }H_2O}{1\text{ mol }H_2O}\right)=1.6\times10^{24}\text{ molec. }H_2O$$

$$1.6\times10^{24}\text{ molec. }H_2O\left(\frac{2\text{ atoms H}}{1\text{ molec. }H_2O}\right)=3.3\times10^{24}\text{ atoms H}$$

- The atomic mass (in *amu*) of an element is numerically equal to the mass (in *g*) of 1 mol of the element
  - ^{12}C → 12 amu 1 mol ^{12}C → 12 g (definitions)
  - C → 12.01 amu 1 mol C → 12.01 g
  - H → 1.008 amu 1 mol H → 1.008 g
  - O → 16.00 amu 1 mol O → 16.00 g
- The molecular (formula) mass (in *amu*) of a compound is numerically equal to the mass (in *g*) of 1 mol of the compound
  - CO_2 → 44.01 amu 1 mol CO_2 → 44.01 g

⇒1 mol of a substance has a fixed mass (can be used to measure moles of substances by weighing them)

Molar Mass (M)

- Mass of a substance per 1 mol of its entities
  - element → atoms (or molecules for H_2, O_2, P_4, ...)
  - molecular compound → molecules
  - ionic compound → formula units
- Units of M → **g/mol**
- $M = m_{particle} \times N_A$

Example:

What is the molar mass of ^{1}H, if the mass of 1 atom ^{1}H is 1.673×10^{-24} g?

$$M = 1.673\times10^{-24}\text{g} \times 6.022\times10^{23}\text{ /mol} = 1.007\text{ g/mol}$$

- M is numerically equal to the atomic, molecular, or formula mass of the substance
  - For elements, M = atomic mass (from per. table)
  - For molecular compounds and molecular elements, M = molecular mass
  - For ionic compounds, M = formula mass

⇒ For compounds and molecular elements, M equals the sum of the molar (atomic) masses of the elements in the formula

Example:

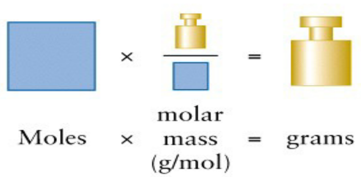
Calculate the molar masses of O_2 and Li_2O.

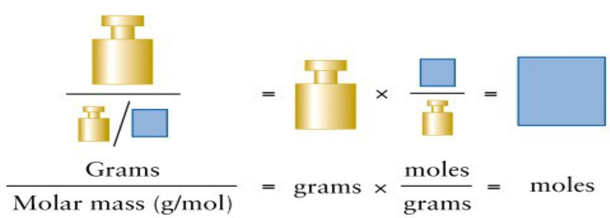
$$M(O_2) = 2\times16.00 = 32.00\text{ g/mol}$$

$$M(Li_2O) = 2\times6.941 + 1\times16.00 = 29.88\text{ g/mol}$$

- M can be used as a conversion factor
- Conversion between moles (n) and mass (m)

$$m = n \times M \quad \leftrightarrow \quad n = m/M$$





- Conversion between moles (n) and masses (m) of elements

Example:

What is the mass of 1.221 mol Kr?

$$m = 1.221\text{ mol} \times 83.80\text{ g/mol} = 102.3\text{ g}$$

Example:

How many moles of atoms are present in 1.23 g of Kr?

$$1.23\text{ g Kr} \times \left(\frac{1\text{ mol Kr}}{83.80\text{ g Kr}}\right) = 1.47\times10^{-2}\text{ mol Kr}$$

- Conversion between moles (n) and masses (m) of compounds (same as for elements)

Example:

Calculate the number of moles of urea, $(NH_2)_2CO$, in 2.3×10^5 kg of this compound.

$M = 2\times14.00 + 4\times1.008 + 1\times12.01 + 1\times16.00 = 60.04$ **g/mol**

$$2.3\times10^5\,\text{kg urea}\times\left(\frac{10^3\,\text{g urea}}{1\,\text{kg urea}}\right)\times\left(\frac{1\,\text{mol urea}}{60.04\,\text{g urea}}\right)$$

$$=3.8\times10^6\,\text{mol urea}$$

- Conversion between masses and number of entities of elements and compounds

Example:

Calculate the number CO_2 molecules and oxygen atoms in **15.8 g** of CO_2.

$M(CO_2) = 12.01 + 2\times16.00 = 44.01$ **g/mol**

$$15.8\,\text{g}\,CO_2\left(\frac{1\,\text{mol}\,CO_2}{44.01\,\text{g}\,CO_2}\right)\left(\frac{6.022\times10^{23}\,\text{molec.}CO_2}{1\,\text{mol}\,CO_2}\right)$$

$$=2.16\times10^{23}\,\text{molec.}CO_2$$

$$2.16\times10^{23}\,\text{molec.}CO_2\left(\frac{2\,\text{atoms O}}{1\,\text{molec.}CO_2}\right)=4.32\times10^{23}\,\text{atoms O}$$

- Conversion between masses of compounds and masses of their elements using chemical formulas (*The subscripts in formulas refer to individual atoms as well as to moles of atoms*)

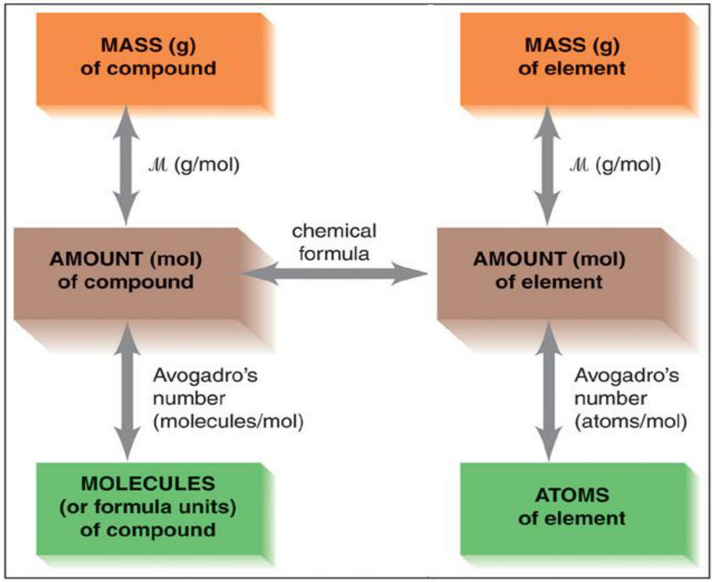
Example: What is the mass of H in **5.00 g** CH_4?

$CH_4 \rightarrow M = 1\times12.01 + 4\times1.008 = 16.04$ **g/mol**

$H \rightarrow M = 1.008$ **g/mol**

$$5.00\,\text{g}\,CH_4\times\left(\frac{1\,\text{mol}\,CH_4}{16.04\,\text{g}\,CH_4}\right)\times\left(\frac{4\,\text{mol H}}{1\,\text{mol}\,CH_4}\right)\times$$

$$\times\left(\frac{1.008\,\text{g H}}{1\,\text{mol H}}\right)=1.26\,\text{g H}$$



Mass Percentage Composition

- Percentage by mass of each element in a compound

$$\textbf{Mass\%} = [m_{element}/m_{compound}]\times 100\%$$

- Calculation of Mass% from chemical formulas
  - Consider 1 mol of a compound

m_{comp} = M of comp

m_{elem} = (# moles of elem in 1 mol of comp)×(M of elem)

Note: The # of moles of the element in 1 mol of the compound equals the # of atoms of the element in the formula of the compound

$$\frac{\text{Mass\% of element}}{} = \left[\frac{(\text{\# atoms of element in formula})(M \text{ of element})}{(M \text{ of compound})}\right]\times 100\%$$

Example:

Calculate the Mass% of O in CO_2.

$CO_2 \rightarrow M = 1\times12.01 + 2\times16.00 = 44.01$ g/mol

$O \rightarrow M = 16.00$ g/mol

$$\text{Mass\% O} = \left(\frac{2\times16.00 \text{ g/mol}}{44.01 \text{ g/mol}}\right)\times 100\% = 72.71\%$$

- Calculation of Mass% from chemical analysis

Example:

Calculate the mass percentage of C in nicotine, if analysis shows that 5.00 g of nicotine contain 3.70 g C, 0.44 g H and 0.86 g N.

$$\text{Mass\% C} = \left(\frac{3.70 \text{ g C}}{5.00 \text{ g nicotine}}\right)\times 100\% = 74.0\%$$