MOLE CONCEPT APPLICATIONS

The mole

- **The mole** (**mol**) - *is the amount of a substance that contains as many elementary entities (atoms, molecules or other particles) as there are atoms in exactly 12 g of the ^{12}C isotope*.

- This number is called ***Avogadro's number*** (N_A) and is equal to 6.022×10^{23}, named after the Italian scientist ***Amedeo Avogadro*** who conducted a series of experiments leading to the "**mole concept**"

- It specifies the number of objects in a fixed mass of substance.

- 1 mole C = 6.022×10^{23} C-12 atoms
- 1 mole H_2O = 6.022×10^{23} H_2O molecules
- 1 mole NaCl = 6.022×10^{23} NaCl “molecules”

  (technically, ionis are compounds not molecules so they are called formula units) 6.022×10^{23} Na^+ ions and 6.022×10^{23} Cl^- ions

- 1 dozen cars = 12 cars
- 1 mole of cars = 6.022×10^{23} cars

- 1 dozen Al atoms = 12 Al atoms
- 1 mole of Al atoms = 6.02×10^{23} atoms

The mole cont'd

- The mass of an atom and a mole are related in that the atomic mass of an element expressed in **amu** is numerically the same as the mass of 1 mole of atoms of the element expressed in **grams**.
- 1 amu = 1.661×10^{-24} g and
- 1 g = 6.022×10^{23} amu

- For atoms, the atomic mass of an element corresponds to the average mass of a single atom in amu and the mass of a mole of atoms in grams.

Learning check

a) Find the number of atoms in 0.500 mol of Al (Ans = 3.01×10^{23} atoms

a) What is the number of moles of S in 1.8×10^{24} S atoms? (Ans = 3.0 mol)

Molar mass

- The Mass of 1 mole (in grams). Equal to the numerical value of the average atomic mass (get from periodic table)

1 mole of C atoms = 12.0 g

1 mole of Mg atoms = 24.3 g

1 mole of Cu atoms = 63.5 g

Molar mass cont'd

- The atomic mass of any substance expressed in grams is the ***molar mass*** (MM) of that substance.
- The ***molar mass*** (MM) of a substance *is the mass of 1 mole of the substance.*

> ➢Note: for all substances, the molar mass in g/mol is numerically equal to the formula weight in amu.

- The atomic mass of iron is 55.85 amu.
- Therefore, the molar mass of iron is 55.85 g/mol.
- Since oxygen occurs naturally as a diatomic, O_2, the molar mass of oxygen gas is 2 times 16.00 g or 32.00 g/mol.

Calculating molar mass

- What is the molar mass of magnesium nitrate, $Mg(NO_3)_2$?

- The sum of the atomic masses is:

$$24.31 + 2(14.01 + 16.00 + 16.00 + 16.00) =$$

$$24.31 + 2(62.01) = 148.33 \text{ amu}$$

- The molar mass for $Mg(NO_3)_2$ is 148.33 g/mol

Mole Calculations

- What is the mass of 2.55×10^{23} atoms of lead?

Answer:

We want grams, we have atoms of lead.

Use Avogadro's number and the molar mass of Pb

$$2.55 \times 10^{23} \cancel{\text{atoms Pb}} \times \frac{1\ \cancel{\text{mol Pb}}}{6.022\times10^{23}\ \cancel{\text{atoms Pb}}} \times \frac{207.2\ \text{g Pb}}{1\ \cancel{\text{mole Pb}}}$$

$$= 87.8\ \text{g Pb}$$

Mole calculations cont'd

- How many O_2 molecules are present in 0.470 g of oxygen gas?

Answer:

We want molecules O_2, we have grams O_2.

Use Avogadro's number and the molar mass of O_2

$$0.470\ \cancel{g\ O_2} \times \frac{1\ \cancel{mol\ O_2}}{32.00\ \cancel{g\ O_2}} \times \frac{6.02\times10^{23}\ \text{molecules}\ O_2}{1\ \cancel{mole\ O_2}}$$

$$= 8.84 \times 10^{21}\ \text{molecules}\ O_2$$

Mass to moles

- How many moles of ethanol are in 10.0 g of ethanol (C_2H_5OH)?

$$10.0\cancel{g\,C_2H_5OH} \times \frac{1\,mol\,C_2H_5OH}{46.1\cancel{g\ C_2H_5OH}} = 0.217\,mol\,C_2H_5OH$$

- What mass (grams) of Zinc iodide can be obtained from 0.0654 mol ZnI_2? = 20.9 g ZnI_2.

Other Names Related to Molar Mass

- ***Molecular Mass/Molecular Weight*****:** If you have a single molecule, mass is measured in **amu** instead of grams. But, the molecular mass is the same numerical value as 1 mole of molecules.
- Thus, Molecular weight (MW) – *is the sum of the atomic weights of all the atoms in a molecule of the substance*.
- ***Formula Mass/Formula Weight (FW)*****:** Same goes for compounds. But again, the numerical value is the same.
- Thus, FW-is the sum of the atomic weights of all atoms in a formula unit of the compound.

Molar mass of molecules and compounds

- Mass in grams of 1 mole equal numerically to the sum of the atomic masses
- 1 mole of $CaCl_2$ = 111.1 g/mol

  1 mole Ca x 40.1 g/mol + 2 moles Cl x 35.5 g/mol

  = 111.1 g/mol $CaCl_2$
- 1 mole of N_2O_4 = 92.0 g/mol
- Prozac, $C_{17}H_{18}F_3NO$, is a widely used antidepressant that inhibits the uptake of serotonin by the brain. Find its molar mass

Calculating the Formula Weight

- Calculate the formula weight of each of the following using a table of atomic weights:

a. Chloroform , $CHCl_3$; = 119.4 amu
b. Iron (III) sulphate, $Fe_2(SO_4)_3$;= 399.9 amu
c. Glucose, $C_6H_{12}O_6$; = ………….
d. Magnesium hydroxide, $Mg(OH)_2$; = ………….

Number of Atoms/Molecules

- How many atoms of Cu are present in 35.4 g of Cu

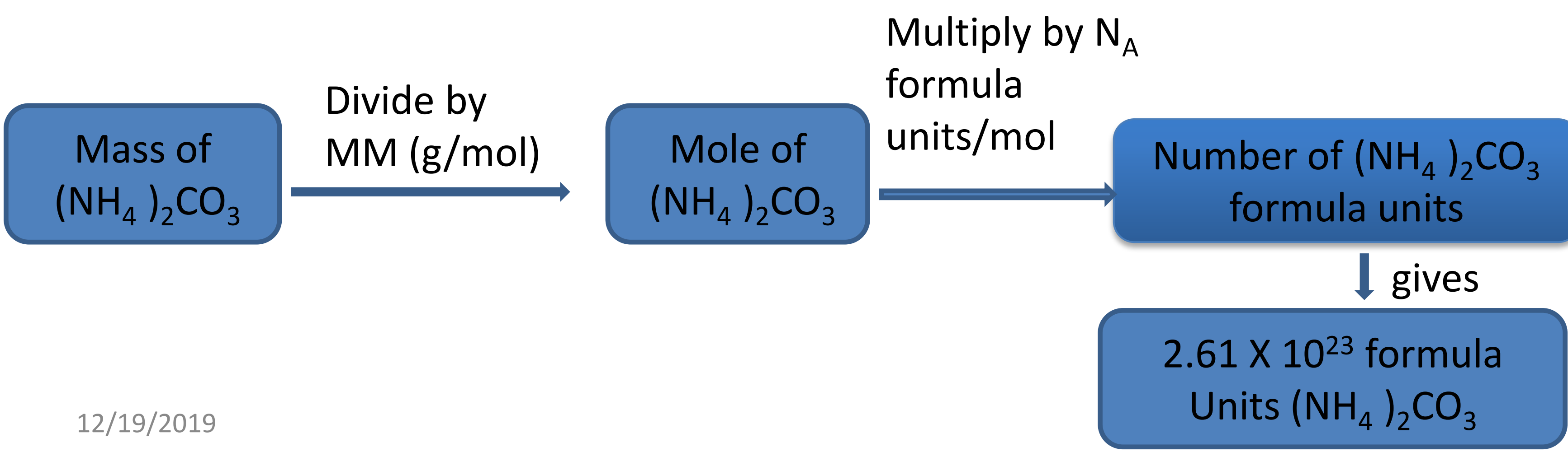
$$35.4\cancel{gCu} \times \frac{1\cancel{molCu}}{63.5\cancel{gCu}} \times \frac{6.022 \times 10^{23}\,atomsCu}{1\cancel{molCu}}$$

$$= 3.4 \times 10^{23}\,atomsCu$$

Qn: How many atoms of K are present in 78.4 g of K?

Problem

- Ammonium carbonate is a white solid that decomposes with warming. Among its uses; it is a component of baking powder, fire extinguishers, and smelling salts. How many formula units are in 41.6 g of ammonium carbonate?



Mass percent composition

- The ***percent composition*** of a compound lists the mass percentages of each element in the cpd.
- The mass percentages from a given formula can be calculated as follows:

$$Mass\,\%\,A = \frac{mass\ of\ A\ in\ the\ whole}{mass\ of\ the\ whole} \times 100\%$$

- For example, the percent composition of water, H_2O is 11% hydrogen and 89% oxygen
- All water contains 11% hydrogen and 89% oxygen by mass.

Calculating mass percent composition

- There are a few steps to calculating the percent composition of a compound. Lets practice using H_2O.
  - Assume you have 1 mole of the compound.
  - One mole of H_2O contains 2 mol of hydrogen and 1 mol of oxygen.
  - 2(1.01 g H) + 1(16.00 g O) = molar mass H_2O
  - 2.02 g H + 16.00 g O = 18.02 g H_2O

Calculating percent composition

- Next, find the percent composition of water by comparing the masses of hydrogen and oxygen in water to the molar mass of water

$$\frac{2.02 \text{ g H}}{18.02 \text{ g } H_2O} \times 100\% = 11.2\% \text{ H}$$

$$\frac{16.00 \text{ g O}}{18.02 \text{ g } H_2O} \times 100\% = 88.79\% \text{ O}$$

Mass Percent Calculation

- The mass percent can be calculated as follows:

$$\text{Mass \% of element X} = \frac{\text{moles of X in formula} \times \text{molar mass of X } \left(\frac{\text{g}}{\text{mol}}\right)}{\text{mass (g) 1 mol of compound}} \times 100$$

➢Note: The individual mass percents of the elements in compound must add up to 100% (within rounding).

➢Consider an example for glucose molecule below.

Mass percent composition cont'd

Example. Glucose ($C_6H_{12}O_6$) is the most important nutrient in the living cell for generating chemical potential energy.

a) What is the mass percent of each element in glucose?

b) How many grams of carbon are in 16.55 g of glucose?

Determining the mass percent of each element

- First determine the mass of 1 mol of $C_6H_{12}O_6$

  = (6 X of C) + (12 X of H) + (6 X of O)

  = (6 x 12.01 g/mol) + (12 x 1.008 g/mol) + (6 x 16.00 g/mol)

  = 180.16 g/mol
- Converting moles of C to grams: There 6 mol C/1 mol glucose, so
- Mass (g) of C

$$= 6 \text{ mol C} \times \frac{12.01 \text{ g C}}{1 \text{ mol C}} = 72.06 \text{ g C}$$

Fraction by mass of C

- The mass fraction of carbon is:

$$\text{Mass fraction of C} = \frac{\text{total mass of C}}{\text{Mass of 1 mol glucose}} = \frac{72.6\text{ g}}{180.16\text{ g}} = 0.4000\text{ g C/g glucose}$$

$$\text{Mass \% of C} = \text{mass fraction of C} \times 100 = 0.4000 \times 100 = 40.00\text{ mass \% C}$$

$$\text{Mass \% of H} = \frac{\text{mol H} \times \text{M of H}}{\text{Mass of 1 mol glucose}} \times 100 = \frac{12\text{ mol H} \times 1.008\text{ g}\frac{\text{H}}{\text{mol H}}}{180.16\text{ g}} \times 100 = 6.714\text{ mass \% H}$$

$$\text{Mass \% 0f O} = \frac{\text{mol O} \times \text{M of O}}{\text{Mass of 1 mol glucose}} \times 100 = \frac{6\text{ mol O} \times 16.00\text{ g}\frac{\text{O}}{\text{mol O}}}{180.16\text{ g}} \times 100 = 53.29\text{ mass \% O}$$

The mass of C

- ❖ Can be found from mass fraction:
- Mass (g) of C = Mass of glucose × mass fraction of C

$$= 16.55 \text{ g glucose} \times \frac{0.4000 \text{ g C}}{1 \text{ g glucose}} = 6.620 \text{ g C}$$

OR,

- ❖ Just multiply the given mass of compound by the ratio of the total mass of element to the mass of 1 mol of compound:

$$\text{Mass (g) C} = 16.55 \text{ g glucose} \times \frac{72.06 \text{ g C}}{180.16 \text{ g glucose}} = 6.620 \text{ g C}$$

Mass cont'd

a) Calculate the mass percentages of the elements in formaldehyde (CH_2O). (40.0% C, 6.73% H, 53.3% O).

b) How many grams of carbon are there in 83.5 g of formaldehyde?

Mass of C = Mass of CH_2O x mass fraction of C

= 83.5 g x 0.400 = 33.4 g C.

H/W

- Ammonium nitrate (NH_4NO_3), is used as a fertilizer and to manufacture explosives. Agronomists base the effectiveness of fertilizers on their nitrogen content.

a) Calculate the mass percentages of the elements in ammonium nitrate.

b) How many grams of N are in 35.8 kg of ammonium nitrate?

Mass Percent Composition Problem

- TNT (trinitrotoluene) is a white crystalline substance that explodes at 240 °C. Calculate the percent composition of TNT, $C_7H_5(NO_2)_3$.
- 7(12.01 g C) + 5(1.01 g H) + 3(14.01 g N + 32.00 g O)

  = …..g $C_7H_5(NO_2)_3$

- 84.07 g C + 5.05 g H + 42.03 g N + 96.00 g O

  = 227.15 g $C_7H_5(NO_2)_3$.

Mass Percent Composition of TNT

$$\frac{84.07 \text{ g C}}{227.15 \text{ g TNT}} \times 100\% = 37.01\% \text{ C}$$

$$\frac{1.01 \text{ g H}}{227.15 \text{ g TNT}} \times 100\% = 2.22\% \text{ H}$$

$$\frac{42.03 \text{ g N}}{227.15 \text{ g TNT}} \times 100\% = 18.50\% \text{ N}$$

$$\frac{96.00 \text{ g O}}{227.15 \text{ g TNT}} \times 100\% = 42.26\% \text{ O}$$

Determining the formula of an unknown compound

- Use the masses of elements in a compound to find its formula.
- The ***empirical formula*** of a compound *is the simplest whole number ratio of moles of each element in the compound.*
- The molecular formula of benzene is C_6H_6
  - The empirical formula of benzene is CH
- The molecular formula of octane is C_8H_{18}
  - The empirical formula of octane is C_4H_9.

Calculating Empirical Formula

- Elemental analysis of a sample of an ionic compound gave the following results: 2.82 g of Na, 4.35 g of Cl, and 7.83 g of O.
- What is the empirical formula and name of the compound?

***Plan*:-**

- Convert masses into integer subscripts i.e. find the number of moles of each element, then construct preliminary formula.

Empirical formula cont'd

Elements	Na	Cl	O
mass	2.82 g	4.35 g	7.83 g
Mass/M	$\frac{2.82 \text{ g Na}}{22.99 \text{ g Na/mol}}$	$\frac{4.35 \text{ g Cl}}{35.45 \text{ g Cl/mol}}$	$\frac{7.83 \text{ g O}}{16.00 \text{ g O/mol}}$
Moles	= 0.123 mol Na	= 0.123 mol Cl	= 0.489 mol O
Preliminary formula	$Na_{0.123}Cl_{0.123}O_{0.489}$		
Divide by the smallest no. of moles	$Na_{\frac{0.123}{0.123}}Cl_{\frac{0.123}{0.123}}O_{\frac{0.489}{0.123}} = Na_{1.00}Cl_{1.00}O_{3.98}$		

∴The empirical formula is $NaClO_4$; Sodium perchlorate

H/W

- An unknown metal M reacts with sulfur to form a compound with formula M_2S_3. If 3.12 g of M reacts with 2.88 g of S, What are the names of M and M_2S_3? (*Hint*: determine number of moles of sulfur and use the formula to find number of moles of M).

- NOTE: In some cases the ratio of the smallest number of moles does not give an integer subscript until when multiplied by a simple whole number.

Empirical Formula from Percent Composition

- We can also use percent composition data to calculate empirical formulas.
- Assume that you have 100 grams of sample.
- Benzene is 92.2% carbon and 7.83% hydrogen, what is the empirical formula.
- If we assume 100 grams of sample, we have 92.2 g carbon and 7.83 g hydrogen.

Empirical Formula from Percent Composition

- Calculate the moles of each element:

$$92.2\ \cancel{\text{g C}} \times \frac{1\ \text{mol C}}{12.01\ \cancel{\text{g C}}} = 7.68\ \text{mol C}$$

$$7.83\ \cancel{\text{g H}} \times \frac{1\ \text{mol H}}{1.01\ \cancel{\text{g H}}} = 7.75\ \text{mol H}$$

- The ratio of elements in benzene is $C_{7.68}H_{7.75}$. Divide by the smallest number to get the formula.

$$C_{\frac{7.68}{7.68}}H_{\frac{7.75}{7.68}} = C_{1.00}H_{1.01} = CH$$

Molecular Formula

- As seen from previous slide , the empirical formula for benzene is CH. This represents the ratio of C to H atoms of benzene.
- The ***molecular formula*** *shows the actual number of moles of each element in 1 mol of the compound.* (some multiple of the empirical formula, $(CH)_n$.
- Benzene has a molar mass of 78 g/mol. Find *n* to find the molecular formula

$$\frac{(CH)_n}{CH} = \frac{78\text{ g/mol}}{13\text{ g/mol}}$$

$n = 6$ and the molecular formula is C_6H_6.

Molecular formula cont'd

- Water, ammonia and methane, for instance have identical empirical and molecular formulas.
- In many other compounds, the molecular formula is a whole number multiple of the empirical formula

$$\text{whole-number multiple(n)} = \frac{\text{molar mass}\left(\frac{\text{g}}{\text{mol}}\right)}{\text{empirical formula mass}\left(\frac{\text{g}}{\text{mol}}\right)}$$

H/W

One of the most widespread environmental carcinogen is benzo[a]pyrene (M = 252.30 g/mol). It is found in coal dust, cigarette smoke, and even in charcoal-grilled meat. Analysis of this hydrocarbon shows 95.21 mass % Carbon and 4.79 mass % Hydrogen. What is the molecular formula of benzo[a]pyrene?

Predicting Amounts of Reactant Consumed or Product Formed

- ***Chemical equation*** -shorthand notation for a chemical reaction, where one substance(s) changes chemically into another substance(s).
- It shows the molar quantity of reactants needed to produce a certain molar quantity of products E.g. $CaCO_3(s) \xrightarrow{\Delta} CaO(s) + CO_2(g)$
- ***Reactants***-starting materials that undergo a chemical change
- ***Products***- ending materials that are produced by a chemical reaction

Limiting Reactant, Theoretical Yield and Percent Yield

- ***The limiting reactant*** (reagent) is the reactant that is (used up first in a reaction) completely consumed in a chemical reaction and limits the amount of product.
- ***The reactant in excess*** is any reactant present in a quantity greater than necessary to react with the quantity of the limiting reactant.
- ***The theoretical yield*** is the amount of product that can be made in a chemical reaction based on the amount of limiting reagent.
- ***The actual yield*** is the amount of product actually obtained from a chemical reaction.

Reaction yield

The actual yield is almost always less than the theoretical yield due to:

1. Incomplete reactions (reversible)-not proceed to completion 100%
2. Insufficient means to collect all the product formed (aqueous solution).
3. Complex reactions - the products can reacts further among themselves or with the reactants to form other products

The Percent Yield

- The percent yield is used by chemists to determine efficiency of the rxn as follows:

$$\% \text{ Yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%$$

- Can be affected by temperature and pressure.
- When working in the laboratory, we measure the initial quantities of reactants in grams, not in the number of molecules.
- In finding the limiting reactant and theoretical yield from initial masses, first convert the masses to amounts in moles.

Limiting Reactant and Theoretical Yield

- Ammonia can be synthesized by the following reaction:
- $2NO(g) + 5H_2(g) \rightarrow 2NH_3(g) + 2H_2O(g)$
- Starting with 86.3 g of NO and 25.6 g H_2, find the theoretical yield of ammonia in grams
- First, find the molar masses of the reacting species

✓ Molar masses: NO = 30.01 g/mol, H_2 = 2.02 g/mol, NH_3, = 17.03 g/mol.

➢ 2 mol NO : 2 mol NH_3 – reaction stoichiometry.

➢ 5 mol H_2 : 2 mol NH_3 – reaction stoichiometry.

The Theoretical Yield cont'd

g NO $\xrightarrow{\frac{1\ \text{mol NO}}{30.01\ \text{g NO}}}$ Mol NO $\xrightarrow{\frac{2\ \text{mol NH}_3}{2\ \text{mol NO}}}$ Mol NH_3

g H_2 $\xrightarrow{\frac{1\ \text{mol H}_2}{2.02\ \text{g H}_2}}$ mol H_2 $\xrightarrow{\frac{2\ \text{mol NH}_3}{5\ \text{mol H}_2}}$ mol NH_3

Smallest amount determines limiting reactant

$\xrightarrow{\frac{17.03\ \text{g NH}_3}{1\ \text{mol NH}_3}}$ g NH_3

Theoretical Yield Cont'd

- The above expressions gives the following

$$86.3\cancel{gNO} \times \frac{1\cancel{molNO}}{30.01\cancel{gNO}} \times \frac{2molNH_3}{2\cancel{molNO}} = 2.8\underline{7}57molNH_3$$

Limiting reactant

Least amount of product

$$25.6gH_2 \times \frac{1\cancel{molH_2}}{2.02\cancel{gH_2}} \times \frac{2molNH_3}{5\cancel{molH_2}} = 5.0\underline{6}93molNH_3$$

$$2.8\underline{7}57\cancel{molNH_3} \times \frac{17.03gNH_3}{1\cancel{molNH_3}} = 49.0gNH_3$$

➢Since NO makes the least amount of product, it is the limiting reactant, and the theoretical yield of ammonia is 49.0 g

H/W

- Ammonia can also be synthesized by the following reaction:

$$3H_2(g) + N_2(g) \rightarrow 2NH_3(g)$$

- What is the theoretical yield of ammonia, in kg, that can be synthesized from 5.22 kg of H_2 and 31.5 kg of N_2?
- Consider the reaction:

$$Cu + 2AgNO_3 \rightarrow Cu(NO_3)_2 + 2Ag$$

- When 10.0 g of copper was reacted with 60.0 g of silver nitrate solution, 30.0 g of silver was obtained. What is the percent yield of silver obtained? Ans: 88.3%

- Titanium metal can be obtained from its oxide according to the following balanced equation:

$$TiO_2(s) + 2C(s) \rightarrow Ti(s) + 2CO(g)$$

- When 28.6 kg of C is allowed to react with 88.2 kg of TiO_2 (79.87 g/mol), 42.8 kg of Ti (47.87 g/mol) is produced. Find the limiting reactant, theoretical yield (kg), and the percent yield.
- TiO_2 is the limiting reactant, 59.2 kg Ti is the theoretical yield and 80.9% is the % yield