Ch09

Formulas

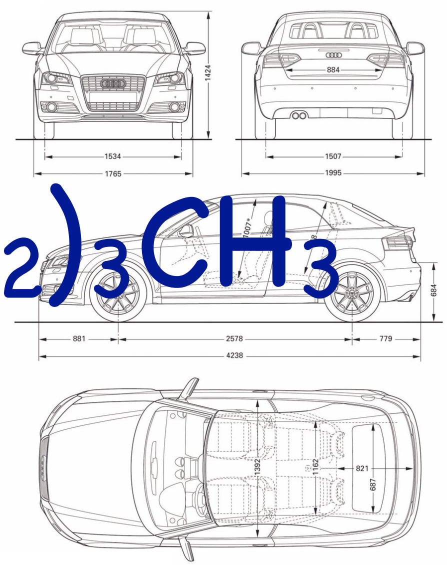
Exploring the molecular blueprint.

How we represent compounds & molecules.

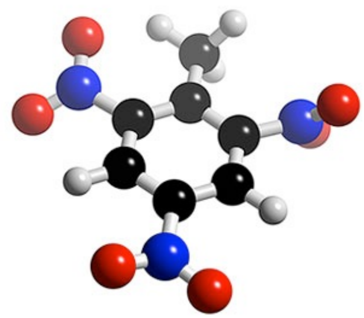
version 1.5

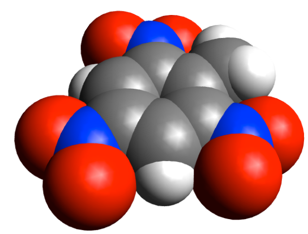
Chemical Formulas

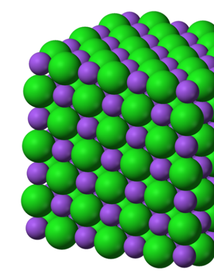
- Molecules & Compounds
  - Compounds are not mixtures.
  - Chemical Bonding
    - covalent vs ionic bonds
    - molecular vs ionic compounds
- Chemical Formula
  - Symbols in Formulas
  - Kinds of chemical formula
    - Identification, Composition
- Composition
  - Molecular Formulas
  - Molecular Weight
  - Percent Composition
- Elemental Analysis
  - You can calculate the percent composition of elements in a molecule from it's formula.
    - You can compare your results with combustion analysis to confirm the identity of a substance.
  - You can calculate the ratio of elements in a compound from elemental analysis.
    - This is not the molecular formula!
    - It's just the ratio. The Empirical Formula
  - You can calculate Molecular Formula form the Empirical formula...
    - Only if you have the molar mass!



$C_6H_2(NO_2)_3CH_3$

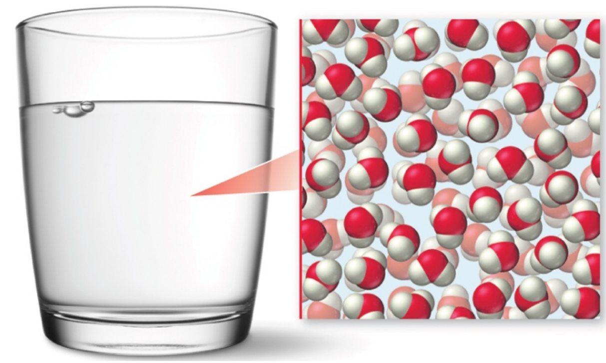


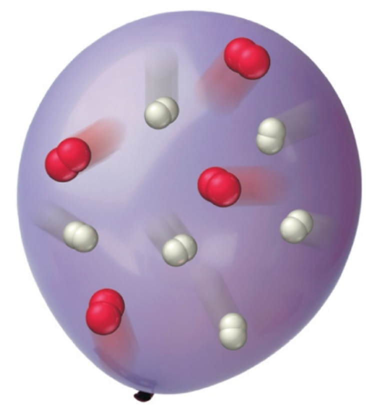




Chemical Bonding

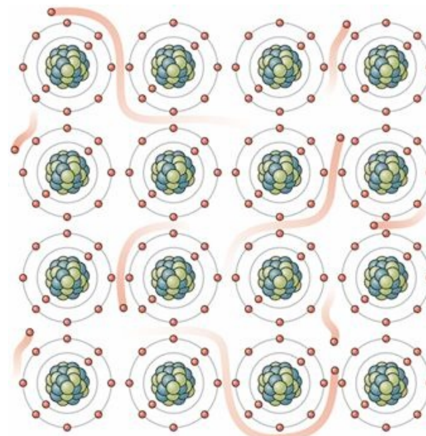
- Bringing elements together to form new compounds.
- Not a mixture, but bonding the elements at the atomic level.
- When you mix hydrogen and oxygen, you don't have a new substance — no new properties are observed.
  - Mixtures are useful, but it's not a reaction.
  - It's just stirring up the particles.
- When you react hydrogen and oxygen, you have a new substance — you see new properties.
  - Water is a compound
    - won't burn
    - liquid at room temperature
    - causes sodium to burn
- The compound forms because the atoms bond to each other.
- All chemical bonding uses electrons to glue atoms to each other
- There are different types of bonding.
    - metallic
    - ionic
    - covalent



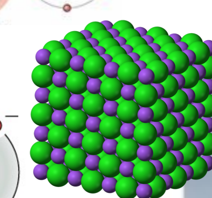


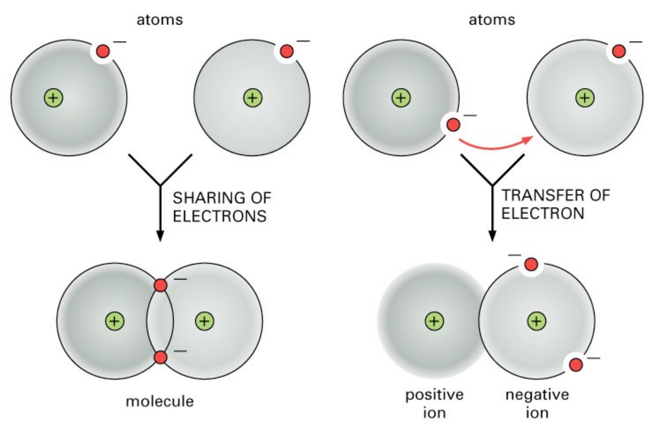
Chemical Bonds

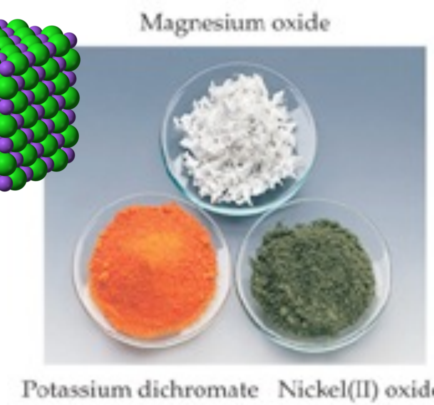
- Metallic Bonding (no non-metals)
  - In pure metals (Fe, Au, Co) or alloys (mixtures of metals) electrons break off and float between the atoms.
  - These free flowing electrons make metals extremely good conductors of electricity.
  - Metal atoms pull on the electrons flowing between them causing the mass to stick together.
  - Metallic bonding does not form compounds.



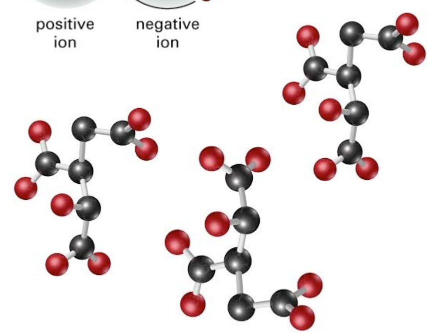
- Ionic Bonding (metal with non-metal)
  - When you mix metals and non-metals electrons break off from metals and are captured by non-metals.
  - This creates positively and negatively charged particles.
  - The particles attract each other, this is an ionic bond.
  - Ionic bonds are extremely strong.
  - These ions clump together in simple, large complexes.
  - Compounds made from ionic bonds are ionic compounds.







- Covalent Bonding (only non-metals)
  - Nonmetals pull on each others electrons.
  - If neither non-metal pulls hard enough to remove the electron from the other, the two end up sharing a pair of electrons.
  - The shared electrons are localized between two atoms, creating a bond between just those two atoms.
  - This produces discrete microscopic structures built of atoms.
  - Particles made of covalent bonds are molecules.
  - Compounds made from covalent bonds are molecular compounds.



Chemical Bonding in Compounds

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  - The shared electrons are localized between two atoms, creating a bond between just those two atoms.
  - Covalent bonding produces discrete microscopic structures built of atoms.
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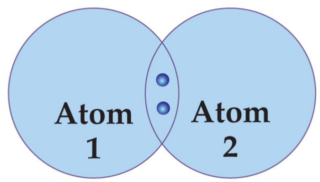
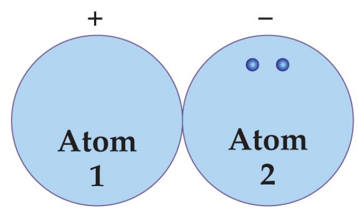


Covalent bond: electrons shared equally



Ionic bond: electron transferred

- Ionic Bonding (metal with non-metal)
  - Ionic bonding creates positively and negatively charged particles.
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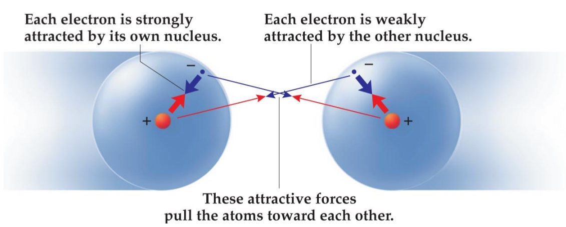
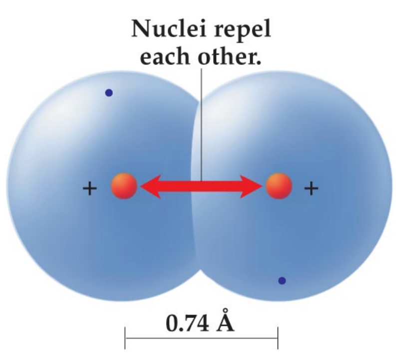
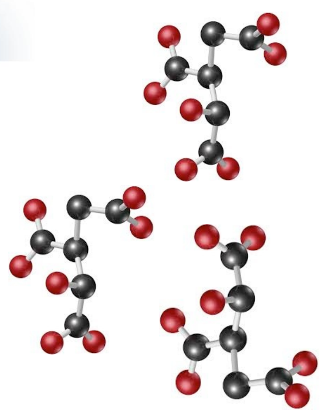
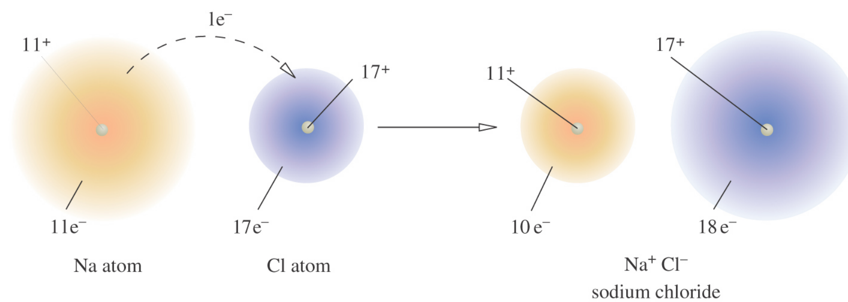
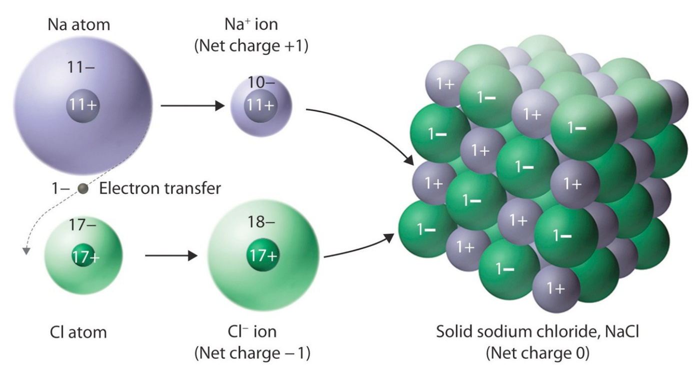
  - These ions clump together in simple, large complexes.
  - Compounds made from ionic bonds are ionic compounds.











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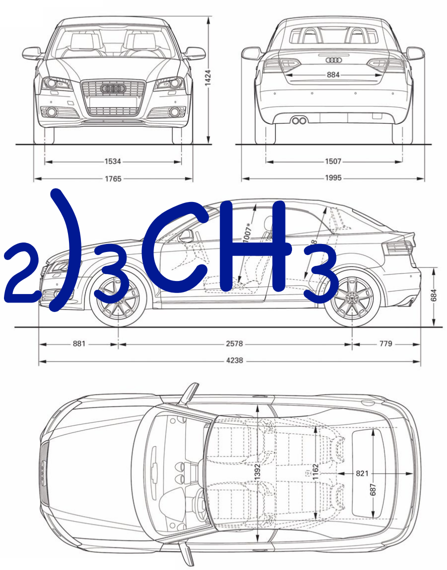

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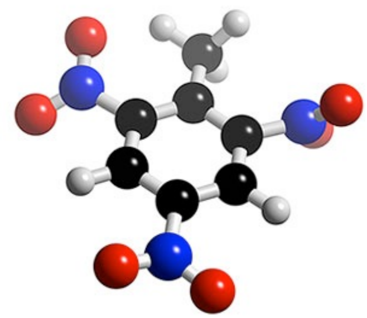
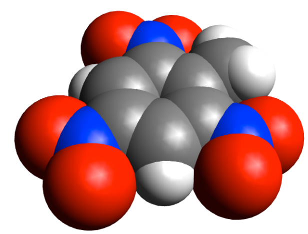
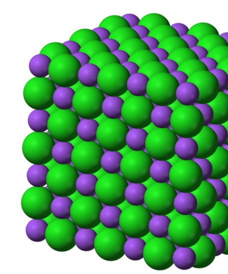




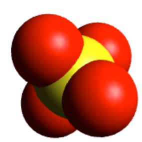


Symbols & Formulas

- We use symbols to represent elements and also to represent atoms of that element.
  - You must memorize the symbols of the first 18 elements! (this is easier than it sounds)
- The order of elements goes from the most metal-like element to the least. Na before C before H before F, etc (we'll talk more about this later)
- We use subscripts to indicate the number of atoms of that element.
  - Subscripts of 1 are omitted.
  - Omitted subscripts mean 1.
- We use superscripts to indicate the net charge (if any) on the entire particle.
  - Superscripts of 0 are omitted.
  - Omitted superscripts are assumed to mean 0.

H_2O

Water is a binary compound, it is a polyatomic molecule composed of 2 hydrogen atoms and 1 oxygen atom. It has a charge of zero.



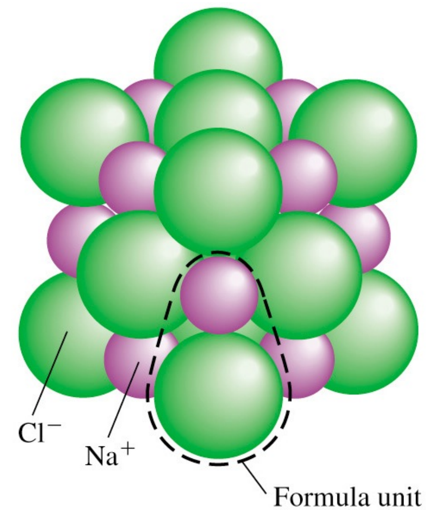
SO_4^{2-}

Sulfate is a binary ion, it is a polyatomic ion composed of 1 sulfur atom and 4 oxygen atoms. It has a charge of minus two.

Au $AlBr_3$ CH_4 Cl^- Na^+ HF Br_2 Al^{3+} NO_2^- Sn $C_6H_8NO_4$ PO_4^{2-}

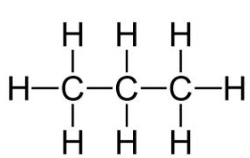
Chemical Formulas in Compounds

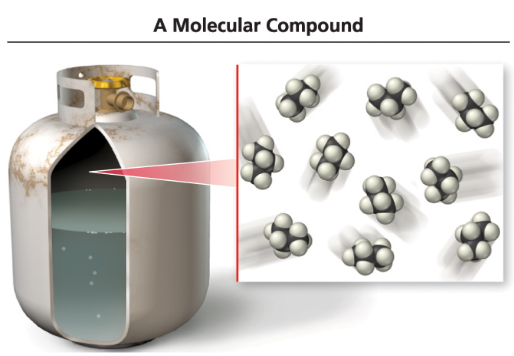
- We use chemical formulas to describe both types of compound.
- There are three kinds of chemical formulas.
- Empirical formula describe the ratio of elements in the compound.
  - Empirical formulas can be applied to molecular or ionic compounds.
  - The smallest whole number ratio of elements is a formula unit.
- Molecular formulas describe the exact number of atoms in each molecule.
  - Molecular formulas can only be used to describe molecular compounds.
- Structural formulas graphically describe the connectivity between atoms.
  - Structural formals can only be used to describe molecular compounds.
  - We'll talk about these in a later chapter.

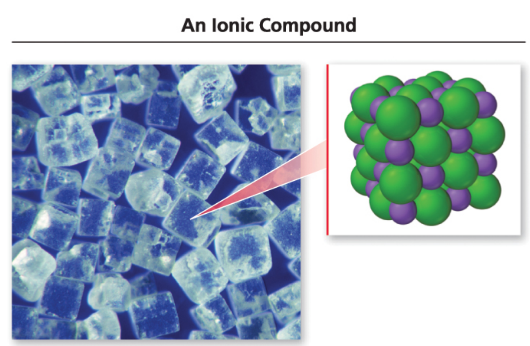


CH_3

C_3H_9







$NaCl$

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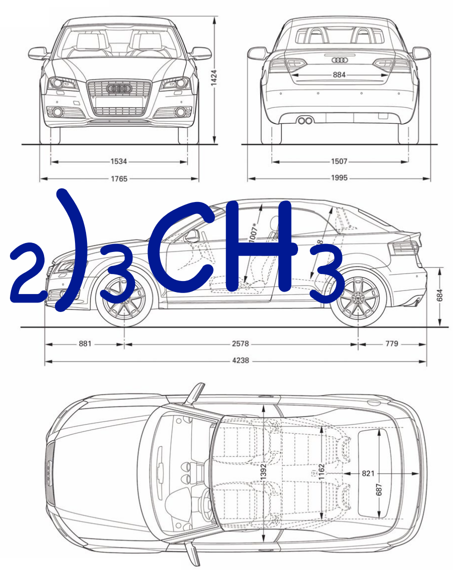
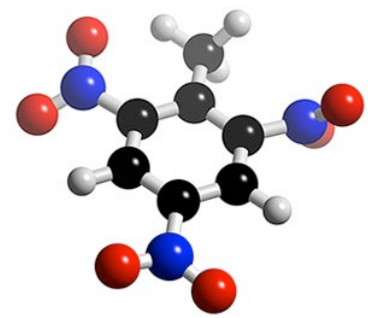
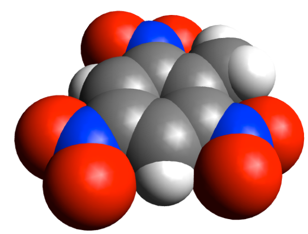
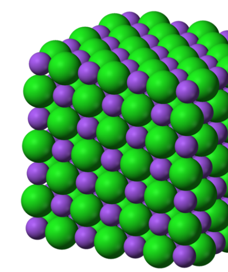
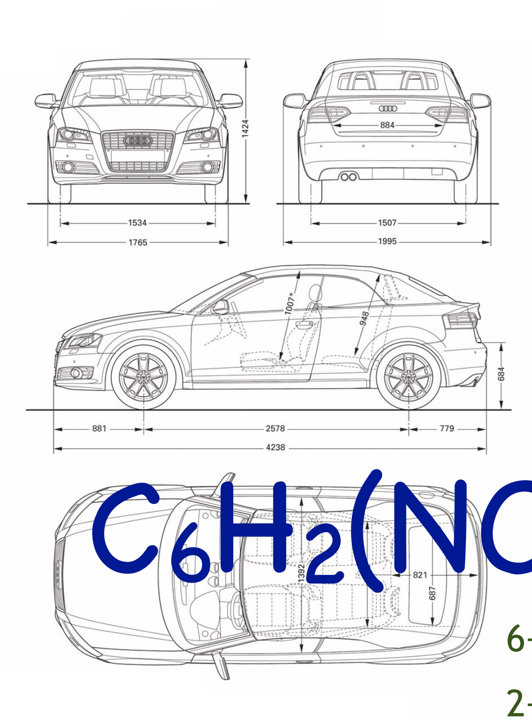








The Molecular Blueprint



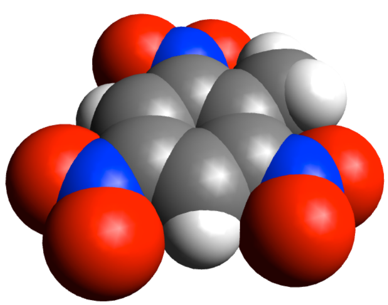
$C_6H_2(NO_2)_3CH_3$

6+1 Carbon Atoms

2+3 Hydrogen Atoms

3 NO_2 Groups

- 3 (3x1) Nitrogen Atoms
- 6 (3x2) Oxygen Atoms



- Chemical Formulas Identify Compounds
  - We use them as shorthand to name of a substance ("Pass me the H_2O")
- Chemical Formulas indicate the composition of a substance.
  - Each element is indicated with it's symbol.
  - The a subscript indicates the total number of atoms of that element.
    - Subscripts of 1 are omitted.
    - Omitted subscripts mean 1.
  - Parenthesis are used to indicate groups of atoms.
- Chemical Formulas may contain hints of the connectivity of the atoms.
- Chemical Formulas may show a CH_3 group of atoms and three NO_2 groups of atoms are bonded to a C_6H_2 group by writing:

$C_6H_2(NO_2)_3CH_3$

instead of: $C_7H_5N_3O_6$

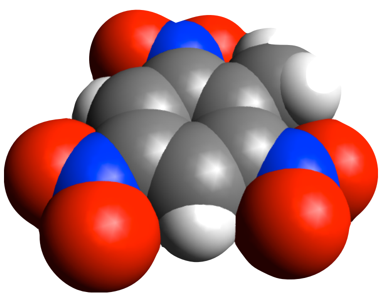
Problem:

You have 2.85 mols of $C_6H_2(NO_2)_3CH_3$ (trinitrotoluene). How many atoms of oxygen do you have?

Solution

mol TNT → molecules TNT → atoms O

6.022×10^{23} singles = 1 mol



1 $C_6H_2(NO_2)_3CH_3$ = 6 O

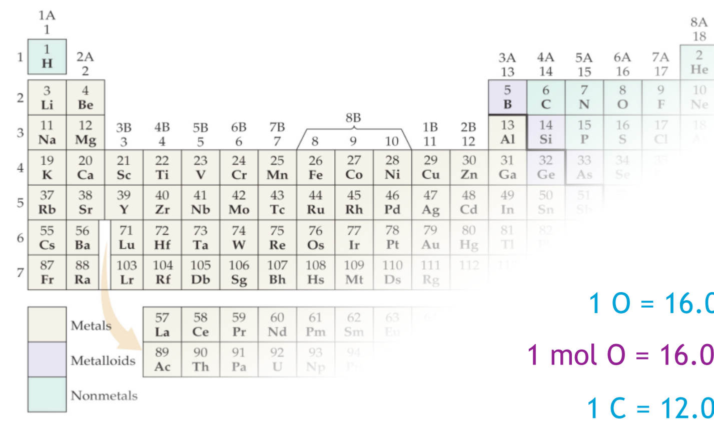
$$2.85 \text{ mol TNT} \cdot \frac{6.022 \times 10^{23} \text{ molecules}}{1 \text{ mol}} \cdot \frac{6 \text{ oxygen atoms}}{1 \text{ molecule TNT}}$$

$$= 1.029762 \times 10^{25} \text{ atoms}$$

$$= \boxed{1.03 \times 10^{25} \text{ atoms O}}$$

Molecular Weight/Molar Mass

- Molar Mass also applies to molecules and compounds.
- We know the atomic weight of elements, what one atoms weighs in amu and what one mole of atoms weigh in grams.
- We can use that information to figure out for compounds what one molecule weighs or one mole of molecules weigh.

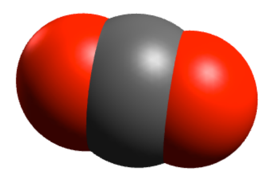


1 O = 16.00 amu

1 mol O = 16.00 g

1 C = 12.01 amu

1 mol C = 12.01 g



What is the molecular weight of CO_2? (in amu)

1 C atom 12.01 amu
2 O atom 32.00 amu (2 × 16.00 amu)

1 CO_2 = 44.01 amu

What is the molar mass of CO_2? (in grams)

1 mol C 12.01 grams
2 mol O 32.00 grams (2 × 16.00 g)

1 mol CO_2 = 44.01 grams

What does 2.57 mol of CO_2 weigh?

$$2.57 \text{ mol } CO_2 \cdot \frac{44.01 \text{ g}}{1 \text{ mol } CO_2} = 113.1057 \text{ g}$$

3 sf   4 sf   113 g CO_2 (3 sf)

How many moles of CO_2 are in 53.256 grams?

$$53.256 \text{ g } CO_2 \cdot \frac{1 \text{ mol } CO_2}{44.01 \text{ g}} = 1.2100886 \text{ mol}$$

5 sf   4 sf   1.210 mol CO_2 (4 sf)

Problem:

Your experiment requires 4.26 mols of magnesium chloride ($MgCl_2$). What mass of magnesium chloride do you weigh out for this experiment?

Solution

Mg 24.31 g/mol

Cl 35.45 g/mol

① Find molar mass of $MgCl_2$

② mol → g

① $1(Mg) = 1(24.31) = 24.31\,g$

$2(Cl) = 2(35.45) = 70.90\,g$

$95.21\,g$

$MgCl_2$ 95.21 g/mol

② $4.26\,mol\,MgCl_2 \cdot \frac{95.21\,g}{1\,mol} = 405.5946\,g$

406 g $MgCl_2$

Problem:

You do an experiment that produces 15.35 grams of nitrogen trioxide (NO_3).

How many moles of NO_3 were produced?

Solution

① Find molar mass of NO_3

② g → mol

N = 14.01 g/mol

O = 16.00 g/mol

① 1 (N) = 1 (14.01) = 14.01 g
3 (O) = 3 (16.00) = 48.00 g
62.01 g

NO_3 62.01 g/mol

② $15.35\,g\ NO_2 \cdot \frac{1\ mol}{62.01\,g} = 0.2475407\,g$

$= 0.2475\,g$

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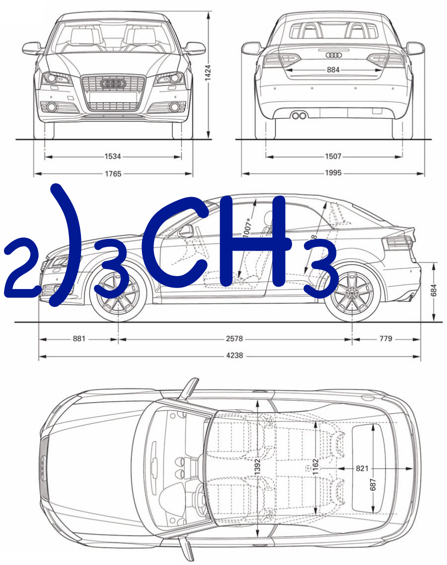

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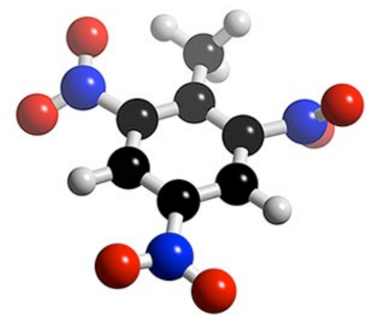
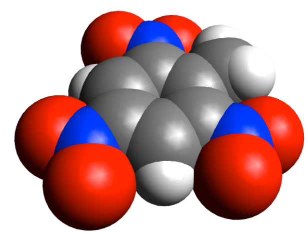
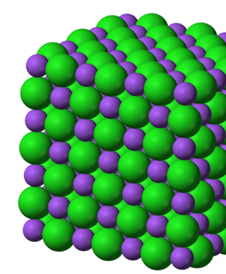
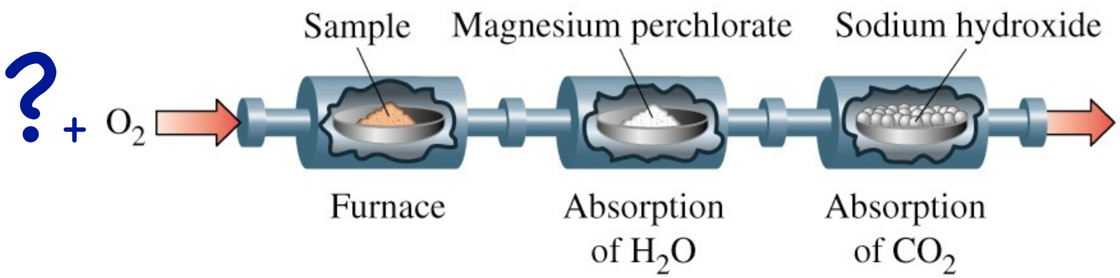




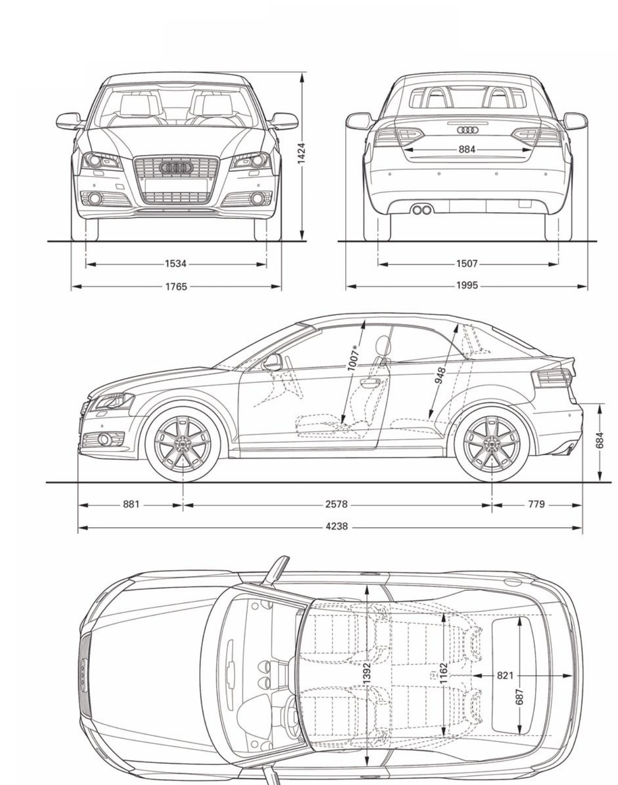


Combustion Analysis / Percent Composition



52.17% C
13.04% H → C_2H_5OH
34.78% O

- A useful technique for analyzing unknown compounds Combustion Analysis, burning an unknown compound and measuring the amounts of products made.
  - This is generally used for organic compounds containing C, H, O.
- By knowing the mass of the unknown and composition of elements in each product, the original amount of each element can be determined.
  - All the original C forms CO_2, the original H forms H_2O, and the original mass of O is found by subtraction.
- This is one way to get the percent composition (also called elemental analysis or elemental composition), of an unknown material.
- Percent Composition is the % by weight of each element in the compound.
- We won't go into the details of combustion analysis calculations, but we will talk using percent composition in different ways.
  - You can calculate percent composition from a chemical formula of a compound you know and compare it to the result of combustion analysis to identify it as the unknown.
  - You can also calculate the chemical formula of an unknown from percent composition, to begin to understand an entirely new compound. (This requires you also know the molecular weight).



Problem:

A detectives observes a substance at a crime scene and hypothesizes that the substance may be phenol. You have a combustion analysis experiment done, here's the report:

You lookup the formula of phenol and find it is C_6H_6O, could the detectives hypothesis be correct?

Report:

C	57.14 %
H	4.796 %
O	38.06 %

Solution

① Find total mass of 1 molecule C_6H_6O

② Divide amount of each element in the molecule by the total mass, to get % of each element.

C_6H_6O

$6(C) = 72.06$ amu
$6(H) = 6.048$ amu
$+ \quad O = 16.00$ amu

94.108

mm = 94.11 amu

$$\%C = \frac{6 \cdot C}{C_6H_6O} = \frac{72.06 \text{ amu}}{94.11 \text{ amu}} \times 100 = 76.57\%$$

$$\%H = \frac{6 \cdot H}{C_6H_6O} = \frac{6.048 \text{ amu}}{94.11 \text{ amu}} \times 100 = 6.427\%$$

$$\%O = \frac{1 \cdot O}{C_6H_6O} = \frac{16.00 \text{ amu}}{94.11 \text{ amu}} \times 100 = 17.00\%$$

The percent compositions do not match.
It's not phenol.

Finding the Empirical Formula

- If you have the elemental analysis, you can figure out the ratio of elements to each other.
- This ratio is the Empirical Formula.
- To find the empirical formula, assume you have 100.00 grams of the substance.
    1. Calculate the grams of each element.
    2. Calculate the moles of each element.
    3. Divide the moles of each element, but the smallest number of moles you find.
    4. You'll get a ratio of each element.
- You may need to multiply it by a small whole number if you get a simple fraction (if you get ½ multiply everything by 2, if you get ⅓ or ⅔ multiply by 3, etc).

Report:
C 57.14 %
H 4.796 %
O 38.06 %

Assume 100.00g of sample:

57.14% of 100.00g is 57.14g C

4.796% of 100.00g is 4.796g H

38.06% of 100.00g is 38.06g O

$$57.14\text{g C} \cdot \frac{1\text{ mol}}{12.01\text{g}} = 4.758 \text{ mol C atoms}$$

$$4.796\text{g H} \cdot \frac{1\text{ mol}}{1.008\text{g}} = 4.758 \text{ mol H atoms}$$

$$38.06\text{g O} \cdot \frac{1\text{ mol}}{16.00\text{g}} = 2.379 \text{ mol O atoms}$$

$$\underset{\text{C}}{\frac{4.758}{2.379}} : \underset{\text{H}}{\frac{4.758}{2.379}} : \underset{\text{O}}{\frac{2.379}{2.379}}$$

$$2 : 2 : 1$$

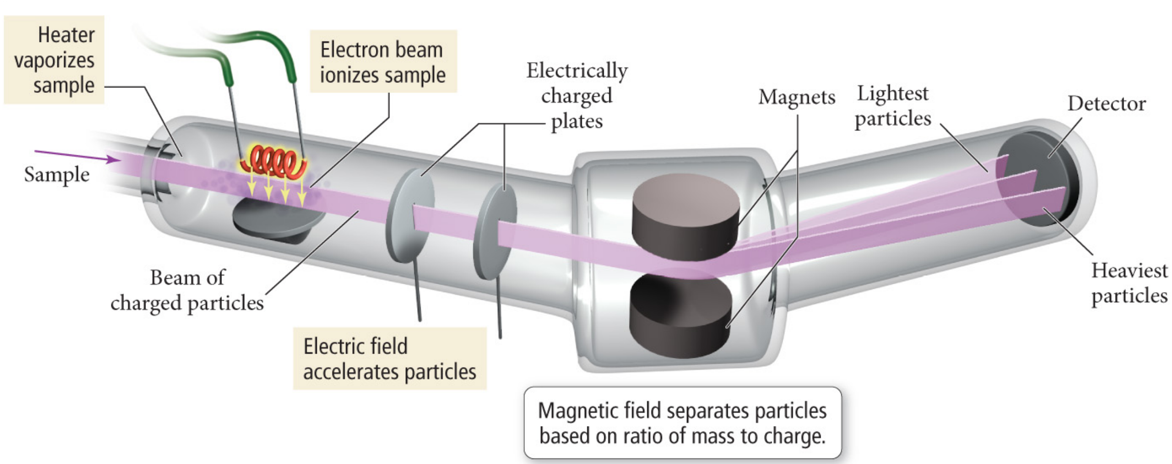
C_2H_2O

Finding the Molar Mass

- The molar mass can only be determined (without already knowing the molecular formula) by experiment.
  - The device we use for this experiment is a mass spectrometer.
  - The material is atomized and shot through a magnet.
  - An electron is knocked of one molecule.
  - By varying the magnetic field you see how much energy is bend the path of the molecule.
  - Once you know how much force it takes to move it, you can get the momentum.
  - If you know the speed and momentum, you can get the mass.

Report:
C 57.14 %
H 4.796 %
O 38.06 %

A mass spectrometer experiment gives us the mass of a molecule like caffeine, the same way it gave us the mass of an atom like copper.



Problem:

A detectives observes a substance at a crime scene. You have a combustion analysis experiment done. You also use a mass spec to find it's molar mass is 126.11 g/mol. What is the molecular formula of this compound?

Report:

C 57.14 %

H 4.796 %

O 38.06 %

Solution

Assume 100.00g of sample:

57.14% of 100.00g is 57.14g C

4.796% of 100.00g is 4.796g H

38.06% of 100.00g is 38.06g O

$57.14\text{g C} \cdot \frac{1\text{ mol}}{12.01\text{g}} = 4.758$ mol C atoms

$4.796\text{g H} \cdot \frac{1\text{ mol}}{1.008\text{g}} = 4.758$ mol H atoms

$38.06\text{g O} \cdot \frac{1\text{ mol}}{16.00\text{g}} = 2.379$ mol O atoms

$$\overset{C}{\frac{4.758}{2.379}} : \overset{H}{\frac{4.758}{2.379}} : \overset{O}{\frac{2.379}{2.379}}$$

2 : 2 : 1

2(C) 24.021
2(H) 2.016
1(O) + 16.00
42.0316

42.04 g/mol

C_2H_2O ← (empirical formula)

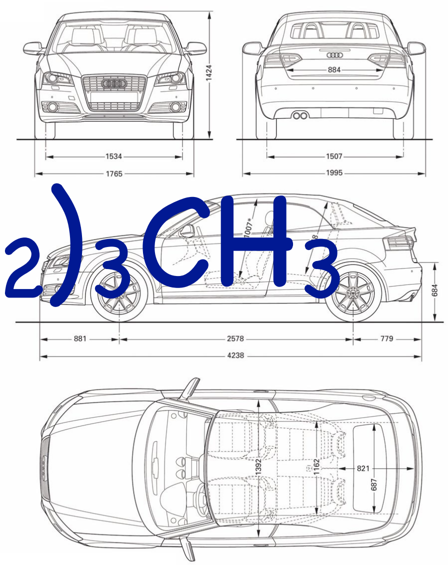
$$\frac{126.11\text{ g}}{42.04\text{ g}} = 2.99976213$$

∴ there are 3 C_2H_2O's in the molecular formula.

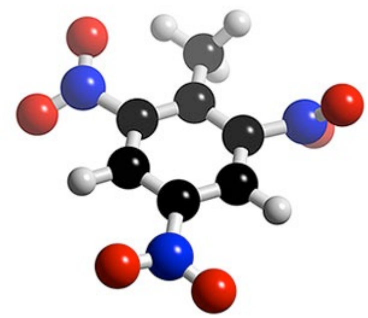
$(C_2H_2O)_3$ = $C_6H_6O_3$

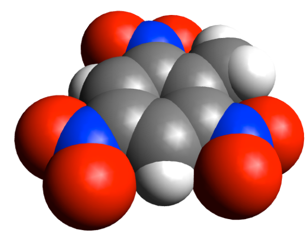
Chemical Formulas

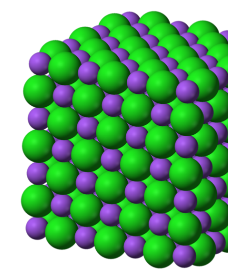
- Molecules & Compounds
  - Compounds are not mixtures.
  - Chemical Bonding
    - covalent vs ionic bonds
    - molecular vs ionic compounds
- Chemical Formula
  - Symbols in Formulas
  - Kinds of chemical formula
    - Identification, Composition
- Composition
  - Molecular Formulas
  - Molecular Weight
  - Percent Composition
- Elemental Analysis
  - You can calculate the percent composition of elements in a molecule from it’s formula.
    - You can compare your results with combustion analysis to confirm the identity of a substance.
  - You can calculate the ratio of elements in a compound from elemental analysis.
    - This is not the molecular formula!
    - It’s just the ratio. The Empirical Formula
  - You can calculate Molecular Formula form the Empirical formula...
    - Only if you have the molar mass!



$$C_6H_2(NO_2)_3CH_3$$





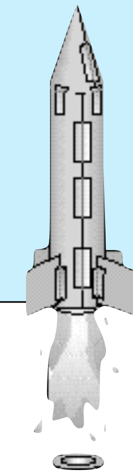


Questions?

How much rocket fuel?

Dinitrogen tetraoxide (N_2O_4) is a rocket fuel. An experiment calls for 6.23 mol of dinitrogen tetraoxide.

How many grams should you weigh out, to get this much fuel? Demonstrate your answer is reliable by providing a dimensional analysis proof.



① Find Molar Mass of N_2O_4

② mol → g

N 14.01 $\frac{g}{mol}$

O 16.00 $\frac{g}{mol}$

① 1 mol N_2O_4

$2(N) = 2(14.01) = 28.02$ g

$4(O) = 4(16.00) = 32.00$ g

$+$ ―――――

60.02 g.

molar mass N_2O_4 60.02 g/mol

②

$6.23 \text{ mol} \cdot \frac{60.02 \text{ g}}{1 \text{ mol}} = 373.9246 \text{ g}$

| 374 g N_2O_4 |

Is it explosive?

Hydrazoic Acid (HN_3) is a colorless, volatile, and extremely explosive liquid. An unknown liquid is found to have the elemental composition 82.27% N and 17.76% H.

Could this unknown be hydrazoic acid? Demonstrate your answer should be trusted by showing how you calculated the elemental composition of hydrazoic acid.

H 1.008 amu / atom
N 14.01 amu / atom

① Find molecular wt of HNH_3

② Find mass of elements in that molecule.

① 1 molecule HN_3

$1(H) = 1 \cdot (1.008) = 1.008$ amu
$3(N) = 3(14.01) = 42.03$ amu
43.038 amu

1 molecule HN_3 weighs 43.04 amu

② $\% H \quad \frac{1(H)}{HN_3} = \frac{1.008 \text{ amu}}{43.04 \text{ amu}} = 0.02342$

2.342 % H

$\% N \quad \frac{3(N)}{HN_3} = \frac{42.03 \text{ amu}}{43.04 \text{ amu}} = 0.9765$

97.65 % N

87.27% N ≠ 97.65% N (It's Not HN_3)