

Numbers and Molecules

Very big and very small

Masses of molecules

- Formula mass
 - Applies to molecules and ionic compounds
 - It is the mass of one formula unit of a compound
- Molecular mass
 - Applies to molecules only
 - It is the mass of a molecule

Mass not weight

- Here we are talking about mass, which is an indication of the amount of material present, not weight, which is a measure of the effect of gravity on the mass.
- An astronaut in orbit is essentially weightless, however, s/he still has the same mass as on Earth.

What is the formula mass?

What is the mass of Iron(III) Sulfate?

Iron(III) Sulfate is $\text{Fe}_2(\text{SO}_4)_3$

In this compound there are:

2 Iron atoms (2×55.85 amu)

3 Sulfur atoms (3×32.07 amu)

12 Oxygen atoms (12×15.9994 amu)

$(2 \times 55.85 \text{ amu}) + (3 \times 32.07 \text{ amu})$

$+ (12 \times 15.9994 \text{ amu}) = 399.91 \text{ amu}$

Molecular masses are calculated the same.

Molecular masses

What is the mass of Dinitrogen Pentoxide?

Dinitrogen Pentoxide is N_2O_5

There are:

2 Nitrogen atoms (2×14.0067 amu)

5 Oxygen atoms (5×15.9994 amu)

$(2 \times 14.0067 \text{ amu}) + (5 \times 15.9994 \text{ amu}) = 108.0104 \text{ amu}$

What about the “real world”?

- Molecular or formula masses are for one unit of the compound.
- In the real world we work with many more than one unit.
- Just as bakers deal with dozens (12) and papermakers deal with reams (512), chemists deal with moles.

What is a mole?

- It is not the thing on Cindy Crawford's lip or a little furry creature.
- It's a counting number defined as being equal to the number of atoms in exactly 12.0000 g of carbon-12. How many is that?

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• 7

Mole

- 1 Mole of anything is equal to 6.0221367×10^{23} of that thing
- This is an extremely large number. It is beyond astronomical numbers.
- How big is this, in tangible terms?

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The size of a mole

- One mole of sand would cover Los Angeles to a depth of ~600 m.



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The size of a mole of money

- If you had one mole of dollars, you could spend \$1,000,000 per second for the rest of your life and only spend 0.4% of the money.



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The size of a mole of stars

- You would need 1,505,500,000,000 galaxies the size of the Milky Way to have one mole of stars.

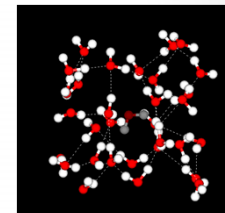


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The size of a mole

- You would need 18 mL of water to have one mole of water molecules.



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• 12

Moles of molecules

- One mole of any molecule is just 6.022×10^{23} of that molecule
- Due to the definition of a mole, one mole of a molecule has the same mass as one molecule but the unit is grams instead of amu.

$$1 \text{ molecule N}_2\text{O}_5 = 108.01 \text{ amu}$$

$$1 \text{ mol N}_2\text{O}_5 = 108.01 \text{ g}$$

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• 13

Moles of atoms in molecules

- The subscripts tell us how many moles of atoms are in one mole of the molecule.
- 1 mole of N_2O_5 contains 2 moles of N and 5 moles of O.

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• 14

Problem solving with moles and molecules

- We use Avogadro's number (6.022×10^{23}) whenever we are moving from the realm of the very large to the realm of the very small or vice versa.
- The most common first step is going to be to convert the number given to moles.
 - This is regardless of whether we are given molecules/atoms or grams.

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• 15

Example Problem 1

- Calculate the number of molecules in 1.000 g of Tetrasulfur Decoxide.

$$\begin{aligned} ? \text{ mol S}_4\text{O}_{10} &= 1.000 \text{ g S}_4\text{O}_{10} \times \frac{1 \text{ mol S}_4\text{O}_{10}}{288.250 \text{ g S}_4\text{O}_{10}} \times \frac{6.022 \times 10^{23} \text{ molc S}_4\text{O}_{10}}{1 \text{ mol S}_4\text{O}_{10}} \\ &= 2.089 \times 10^{21} \text{ molc S}_4\text{O}_{10} \end{aligned}$$

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• 16

Example Problem 2

- What is the mass, in grams, of 1.648×10^{22} formula units of Lead(IV) Dichromate?

$$\begin{aligned} ? \text{ g Pb}(\text{Cr}_2\text{O}_7)_2 &= 1.648 \times 10^{22} \text{ f.u. Pb}(\text{Cr}_2\text{O}_7)_2 \times \frac{1 \text{ mol Pb}(\text{Cr}_2\text{O}_7)_2}{6.022 \times 10^{23} \text{ f.u. Pb}(\text{Cr}_2\text{O}_7)_2} \\ &\quad \times \frac{639.17 \text{ g Pb}(\text{Cr}_2\text{O}_7)_2}{1 \text{ mol Pb}(\text{Cr}_2\text{O}_7)_2} = 17.49 \text{ g Pb}(\text{Cr}_2\text{O}_7)_2 \end{aligned}$$

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• 17

Example Problem 3

- Calculate the number of Nitrogen atoms in 15.00 g of Ammonium Azide.

$$\begin{aligned} ? \text{ at N} &= 15.00 \text{ g NH}_4\text{N}_3 \times \frac{1 \text{ mol NH}_4\text{N}_3}{60.0586 \text{ g NH}_4\text{N}_3} \times \frac{4 \text{ mol N}}{1 \text{ mol NH}_4\text{N}_3} \\ &\quad \times \frac{6.022 \times 10^{23} \text{ at N}}{1 \text{ mol N}} = 6.016 \times 10^{23} \text{ at N} \end{aligned}$$

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• 18

Percent Composition

- All compounds have a certain percent composition
- Percent composition is the percent of the total mass that each element has in the compound.

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• 19

Example: H₂O

- The mass of one mole of water is 18.015 g.
- Of that mass 2x1.008 g is Hydrogen and 15.9994 g is oxygen.

- The percent of Hydrogen is:

$$\frac{2 \times 1.008}{18.015} \times 100 = 11.19 \%$$

- Oxygen is the rest (100.0-11.19=88.81%)

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• 20

Empirical Formula

- The empirical formula gives the lowest whole number ratio of atoms in a compound.
- The chemical formula for ionic compounds is an empirical formula.
- For covalent compounds, the molecular formula is a whole number multiple of the empirical formula

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• 21

Examples

- For water (H₂O) the empirical formula is the same as the molecular formula (multiplier is 1).
- For sugar (C₆H₁₂O₆) the empirical formula is CH₂O (multiplier is 6).
- For Hydrogen Peroxide (H₂O₂) the empirical formula is HO (multiplier is 2).

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• 22

Why empirical formulas?

- The empirical formula is relatively easy to calculate.
- If we can find the molar mass, which we usually can, we can then find the molecular formula.

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How to calculate empirical formulas

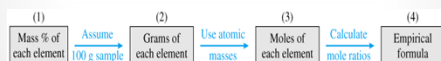
- We need the percent composition, which can be experimentally determined.
- The percent composition allows us to calculate the ratio of moles of atoms in the compound.

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• 24

How to calculate empirical formulas

1. Assume 100.00 g of compound. Then the percentages can be thought of as masses.
2. Convert the mass of each element present to moles
3. Divide all of the moles by the lowest number of moles.
4. If necessary, multiply the quotients from 3 by a whole number to get whole numbers.



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Example

- A compound is composed of 63.15% C, 5.30% H and 31.55% O. What is the empirical formula?

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Assume 100.00 g of compound

- This means we have 63.15 g C, 5.30 g H and 31.55 g O.

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Convert masses to moles

$$63.15 \text{ g C} \times \frac{1 \text{ mol C}}{12.011 \text{ g C}} = 5.258 \text{ mol C}$$

$$5.30 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 5.25 \text{ mol H}$$

$$31.55 \text{ g O} \times \frac{1 \text{ mol O}}{15.9994 \text{ g O}} = 1.972 \text{ mol O}$$

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• 28

Divide all the moles by the lowest

$$\text{For C: } \frac{5.258}{1.972} = 2.666$$

$$\text{For H: } \frac{5.25}{1.972} = 2.662$$

$$\text{For O: } \frac{1.972}{1.972} = 1.000$$

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• 29

Is there more?

- We do not have whole numbers (or within ± 0.1 of a whole number) so we must multiply by a whole number to get close to whole numbers.
- If we have 0.25 or 0.75 we multiply by 4, if we have 0.33 or 0.66 we multiply by 3, if we have 0.50 we multiply by 2.
- In this case we have 0.66 so we multiply all of them by 3.

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• 30

Multiplication by a constant

For C: $2.666 \times 3 = 8$

For H: $2.662 \times 3 = 8$

For O: $1.000 \times 3 = 3$

This gives an empirical formula of $C_8H_8O_3$.

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• 31

What about molecular formulas?

- To get the molecular formula, we need to know the molar mass.
- We also need to calculate the empirical mass.
- Divide the molecular mass by the empirical mass.
- Multiply the subscripts by the number from above, which should be an integer.

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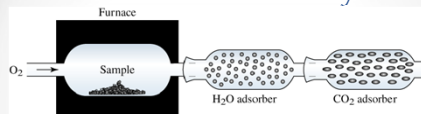


- For this empirical formula the mass is 152.15 g.
- The molar mass is 152.15 g.
- Division gives: $\frac{152.15}{152.15} = 1$
- This indicates that the empirical and molecular formulas are the same, $C_8H_8O_3$.

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• 33

Combustion Analysis



In combustion analysis, a compound is burned and the gases produced are analyzed. The mass of water vapor and carbon dioxide tells us the mass of C and H in the compound. Oxygen is determined by difference.

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• 34

How to calculate

- Grams of CO_2 gives us grams and moles of C.
- Grams of H_2O gives us grams and moles of H.
- Grams and moles of oxygen is found from the difference between the mass of the sample and the mass of C and H.
- Then find lowest whole number ratio of moles to get empirical formula.

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• 35

Example

0.1145 g of a compound containing C, H and O is burned. 0.1624 g of CO_2 and 0.0997 g of H_2O are produced. What is the empirical formula for this compound? If the molar mass is 62.07 g, what is the molecular formula?

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• 36

Convert masses to masses

$$0.1624 \text{ g CO}_2 \times \frac{1 \text{ mol CO}_2}{44.010 \text{ g CO}_2} \times \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} =$$

$$0.003690 \text{ mol C} \times \frac{12.011 \text{ g C}}{1 \text{ mol C}} = 0.04432 \text{ g C}$$

$$0.0997 \text{ g H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{18.015 \text{ g H}_2\text{O}} \times \frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}} =$$

$$0.01107 \text{ mol H} \times \frac{1.008 \text{ g H}}{1 \text{ mol H}} = 0.01115 \text{ g H}$$

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• 37

Find Oxygen by difference

$$0.1145 \text{ g} - 0.04432 \text{ g C} - 0.01115 \text{ g H} = 0.05903 \text{ g O}$$

$$0.05903 \text{ g O} \times \frac{1 \text{ mol O}}{15.9994 \text{ g O}} = 0.003689 \text{ mol O}$$

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• 38

Find mole ratios

$$\frac{0.003690}{0.003689} = 1.0003$$

The empirical formula is CH₃O

$$\frac{0.01107}{0.003689} = 3.001$$

The empirical mass is 31.04.

$$\frac{0.003689}{0.003699} = 1.000$$

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• 39

Molecular formula

$$\frac{\text{molar mass}}{\text{empirical mass}} = \frac{62.07}{31.04} = 1.9996778 = 2$$

The molecular formula is C₂H₆O₂.

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• 40