

Chemical Calculations

Molecular mass: The sum of the atomic masses of all the atoms in a molecule of a substance.

Formula mass: The sum of the atomic masses of all the atoms in a formula unit of a substance.

For molecules: Molecular weight and formula weight are the same.

For ionic compounds: Only the term formula weight applies.

Mole: (mol)

One mole of a substance is the quantity of that substance that contains as many elemental entities as the number of atoms in exactly 12.000 g of Carbon-12. That number is called Avogadro's number (N_A). It is numerically equal to 6.0221367×10^{23} . A mole is just a counting number like a dozen or a ream or a pair. When talking about a mole of something you must specify the formula unit of what you are using. 1 mol O is 6.022×10^{23} atoms of oxygen. 1 mol O_2 is 12.044×10^{23} atoms of oxygen.

Molar Mass: The mass of one mole of substance.

The molar mass in g/mol is numerically equivalent to the molecular or formula mass in amu.

Examples:

1. How many formula units are in 254.2 g of Lead(II) Oxide?

The formula for Lead(II) Oxide is PbO which results in a molar mass of 223.19 g (207.19 g + 15.9994 g).

$$254.2 \text{ g PbO} \times \frac{1 \text{ mol PbO}}{223.19 \text{ g PbO}} \times \frac{6.022 \times 10^{23} \text{ formula units PbO}}{1 \text{ mol PbO}} = 6.859 \times 10^{23} \text{ formula units PbO}$$

2. 3.42×10^{22} molecules of water has what mass in grams?

Water has the formula H_2O so it has a molar mass of 18.0153 g ($2 \times 1.0079 \text{ g} + 15.9994 \text{ g}$).

$$3.42 \times 10^{22} \text{ molecules } H_2O \times \frac{1 \text{ mole } H_2O}{6.022 \times 10^{23} \text{ molecules } H_2O} \times \frac{18.0153 \text{ g } H_2O}{1 \text{ mole } H_2O} = 1.02 \text{ g } H_2O$$

Mass percentages: The percentage by mass of all the elements in a compound.

$$\text{mass \% of A} = \frac{\text{mass of A in the sample}}{\text{mass of the sample}} \times 100\%$$

The sum of the percentages for a compound must equal 100%.

Determining chemical formulas

Empirical formula: a formula for a compound that shows the lowest whole number ratio of the elements in the compound.

Empirical formula for water: H₂O

Empirical formula for hydrogen peroxide: HO (H₂O₂)

Empirical formula for glucose: CH₂O (C₆H₁₂O₆)

Empirical formula for ribose: CH₂O (C₅H₁₀O₅)

Determining the empirical formula from mass percentages...

1. Assume 100.00 g of compound. This converts the percentages directly to masses of the elements.
2. Convert the mass of each element to moles of that element.
3. Divide each of the moles by the smallest.
4. If you do not get a series of integers (± 0.1) from step 3. Multiply each of the values by a factor to get everything to integers (± 0.1). This factor will usually be about 2 or 3, but it may be larger.

Determining molecular formulas:

1. Find the empirical formula.
2. Find the empirical mass (the mass of one empirical formula unit).
3. Divide the molar mass by the empirical mass. This should be an integer.
4. Multiply this integer by all the subscripts in the formula.

For compounds containing the elements C, H, and O, the percentages can be determined by combustion. Combustion itself gives carbon dioxide, which gives the percentage of C, and water, which gives the percentage of H. Percentage of O is determined by difference.

Example:

A compound contains 62.04% C, 10.41% H, and the rest is Oxygen. What is the empirical formula for this compound?

Solution:

Assume there is 100.00 g of the compound

$$100.00 \text{ g cpd} \times \frac{62.04 \text{ g C}}{100 \text{ g cpd}} \times \frac{1 \text{ mol C}}{12.011 \text{ g C}} = 5.165 \text{ mol C}$$

$$100.00 \text{ g cpd} \times \frac{10.41 \text{ g H}}{100 \text{ g cpd}} \times \frac{1 \text{ mol H}}{1.0079 \text{ g H}} = 10.32 \text{ mol H}$$

$$100.00 \text{ g cpd} \times \frac{27.55 \text{ g O}}{100 \text{ g cpd}} \times \frac{1 \text{ mol O}}{15.9994 \text{ g O}} = 1.722 \text{ mol O}$$

The smallest of these is 1.722 mol so we divide all the numbers by that one.

$$\frac{5.167 \text{ mol C}}{1.722 \text{ mol}} = 3.001 \approx 3$$

$$\frac{10.32 \text{ mol H}}{1.722 \text{ mol}} = 5.993 \approx 6$$

$$\frac{1.722 \text{ mol O}}{1.722 \text{ mol}} = 1.000 \approx 1$$

Therefore the empirical formula is $\text{C}_3\text{H}_6\text{O}$.

If the molar mass of this compound is $116.16 \text{ g mol}^{-1}$, what is the molecular formula?

$$\frac{\text{Molar mass}}{\text{Empirical mass}} = \frac{116.16 \text{ g mol}^{-1}}{58.08 \text{ g mol}^{-1}} = 2$$

So the molecular formula is twice the empirical formula, $\text{C}_6\text{H}_{12}\text{O}_2$.