

# Empirical Formula and Molecular Formula Calculations



## Simplest formula calculations

Q- a compound is found to contain the following % by mass: 69.58% Ba, 6.090% C, 24.32% O. What is the simplest (i.e. empirical) formula?

**Step 1:** imagine that you have 100 g of the substance. Thus, % will become mass in grams. E.g. 69.58 % Ba becomes 69.58 g Ba. (Some questions will give grams right off, instead of %)

**Step 2:** calculate the # of moles ( $\text{mol} = \text{g} \div \text{g/mol}$ )

**Step 3:** express moles as the simplest ratio by dividing through by the lowest number.

**Step 4:** write the simplest formula from mol ratios.

## Simplest formula: sample problem

Q- 69.58% Ba, 6.090% C, 24.32% O.

What is the empirical (a.k.a. simplest) formula?

1: 69.58 g Ba, 6.090 g C, 24.32 g O

2: Ba:  $69.58 \text{ g} \div 137.33 \text{ g/mol} = 0.50666 \text{ mol Ba}$

C:  $6.090 \text{ g} \div 12.01 \text{ g/mol} = 0.50708 \text{ mol C}$

O:  $24.32 \text{ g} \div 16.00 \text{ g/mol} = 1.520 \text{ mol O}$

3:

	Ba	C	O
mol	0.50666	0.50708	1.520
mol (reduced)	0.50666/ = 1	0.50708/ = 1.001	1.520/ = 3.000

4: the simplest formula is  $\text{BaCO}_3$

## Mole ratios and simplest formula

Given the following mole ratios for the hypothetical compound  $\text{AxBy}$ , what would x and y be if the mol ratio of A and B were:

A = 1 mol, B = 2.98 mol

A = 1.337 mol, B = 1 mol

A = 2.34 mol, B = 1 mol

A = 1 mol, B = 1.48 mol

- A compound consists of 29.1 % Na, 40.5 % S, and 30.4 % O. Determine the simplest formula.
- A compound is composed of 7.20 g carbon, 1.20 g hydrogen, and 9.60 g oxygen. Find the empirical formula for this compound
- 6. Try questions 3 - 6 on page 189.

## Molecular formula calculations

- There is one additional step to solving for a molecular formula. First you need the molar mass of the compound. E.g. in Q2, the molecular formula can be determined if we know that the molar mass of the compound is 150 g/mol.
- First, determine molar mass of the simplest formula. For  $\text{CH}_2\text{O}$  it is 30 g/mol ( $12+2+16$ ).
- Divide the molar mass of the compound by this to get a factor:  $150 \text{ g/mol} \div 30 \text{ g/mol} = 5$
- Multiply each subscript in the formula by this factor:  $\text{C}_5\text{H}_{10}\text{O}_5$  is the molecular formula. (models)

Q- For OF, give the molecular formula if the compound is 70 g/mol

- Combustion analysis gives the following: 26.7% C, 2.2% hydrogen, 71.1% oxygen. If the molecular mass of the compound is 90 g/mol, determine its molecular formula.
- What information must be known to determine
  - the empirical formula of a substance?
  - the molecular formula of a substance?
- A compound's empirical formula is  $\text{CH}$ , and it weighs 104 g/mol. Give the molecular formula.
- A substance is decomposed and found to consist of 53.2% C, 11.2% H, and 35.6% O by mass. Calculate the molecular formula of the unknown if its molar mass is 90 g/mol.

## Assignment

- Calculate the percentage composition of each substance: a)  $\text{SiH}_4$ , b)  $\text{FeSO}_4$
- Calculate the simplest formulas for the compounds whose compositions are listed:
  - carbon, 15.8%; sulfur, 84.2%
  - silver, 70.1%; nitrogen, 9.1%; oxygen, 20.8%
  - K, 26.6%; Cr, 35.4%, O, 38.0%
- The simplest formula for glucose is  $\text{CH}_2\text{O}$  and its molar mass is 180 g/mol. What is its molecular formula?

- Determine the molecular formula for each compound below from the information listed.
 

substance	simplest formula	molar mass(g/mol)
a) octane	$\text{C}_4\text{H}_9$	114
b) ethanol	$\text{C}_2\text{H}_6\text{O}$	46
c) naphthalene	$\text{C}_5\text{H}_4$	128
d) melamine	$\text{CH}_2\text{N}_2$	126
- The percentage composition and approximate molar masses of some compounds are listed below. Calculate the molecular formula of each
 

percentage composition	molar mass(g/mol)
64.9% C, 13.5% H, 21.6% O	74
39.9% C, 6.7% H, 53.4% O	60
40.3% B, 52.2% N, 7.5% H	80