

Calculation of Empirical Formulae and Molecular Formulae

Definition: The empirical formula for a compound gives the ratio of different elements in that compound. The molecular formula gives the *actual* number of each atom present in the compound.

Problem: Glucose is found to contain 40.0% C, 6.67% H by mass, and it has a molar mass of 180.16 g/mol. What are the empirical and the molecular formula for glucose?

Step 1: The missing $(100 - 40.0 - 6.67) = 53.33\%$ comes from **oxygen**.

Step 2: Assume we have 100.0 g of glucose. How many moles would we have of each element?

$$\begin{array}{l} \text{C: } \frac{40.0 \text{ g}}{12.0 \text{ g/mol}} = 3.33 \text{ mol} \qquad \text{H: } \frac{6.67 \text{ g}}{1.01 \text{ g/mol}} = 6.60 \text{ mol} \\ \text{O: } \frac{53.3 \text{ g}}{16.0 \text{ g/mol}} = 3.33 \text{ mol} \end{array}$$

So our formula is in the ratio 3.33 : 6.60 : 3.33.

Step 3: How can we get whole numbers from this? Find the least common element, set this to 1. Then see what you get- in this case:

$$\begin{array}{l} \text{Set carbon to unity (1), then} \quad \text{no. of H} = \frac{6.60}{3.33} = 1.98 \text{ (close to 2)} \\ \qquad \qquad \qquad \qquad \qquad \qquad \text{no. of O} = \frac{3.33}{3.33} = 1.00 \end{array}$$

So the empirical formula for glucose is CH_2O .*

If this process leads to numbers that are not close to integers, then try setting the least common element to 2 or 3.

Step 4. Find the molecular formula. The molar mass = 180.16 g/mol for glucose. For CH_2O the molar mass = 30.03 g/mol, \Rightarrow glucose has $180.16/30.03 = 6$ units. So we have $(\text{CH}_2\text{O})_6$, i.e., the molecular formula for glucose is $\text{C}_6\text{H}_{12}\text{O}_6$.

Note: Most molecular formulae only have 1, 2 or 3 units- but 6 is possible!

Practice problems†:

Glycerol: A by-product of soap-making, this has a molar mass of 92.10 g/mol. It contains 39.1% C, 8.70% H by mass. Find the empirical & molecular formulae.

Tyrosine: An essential amino acid in many living systems. Molar mass 181.19, contains 59.7% C, 6.08% H, 7.73% N by mass. Find empirical & molecular formulae.

* Note that this is equal to carbon + water, hence the name for compounds of this type as *carbohydrates*.

† For answers see the Aldrich or Lancaster catalogue.