

Empirical Formulas

How can the chemical formulas of a compound be determined?

Why?

Scientists use chemical formulas as a shorthand method of communicating with each other about the make-up and structure of compounds. There are several types of formulas that are used to convey different types of information. This activity will compare two types of useful formulas.

Model 1 – Empirical Formula

Compound Name	Molecular Formula	Ratio of Carbon Atoms to Hydrogen Atoms	Lowest Whole Number Ratio of Carbon Atoms to Hydrogen Atoms	Empirical Formula
Methane	CH ₄	1:4	1:4	CH ₄
Ethene (ethylene)	C ₂ H ₄	2:4	1:2	CH ₂
Propene	C ₃ H ₆			CH ₂
Ethyne (acetylene)	C ₂ H ₂	2:2	1:1	CH
Benzene	C ₆ H ₆			CH
1,3-butadiene	C ₄ H ₆			C ₂ H ₃
Propane	C ₃ H ₈			C ₃ H ₈

1. Consider the information in Model 1. How are the columns “ratio of carbon atoms to hydrogen atoms” and “lowest whole number ratio of carbon atoms to hydrogen atoms” related?
2. Complete the table in Model 1 by filling in all of the blank spaces.
3. Which set of ratios in Model 1 is most closely related to the empirical formulas of the compounds—the ratio of the carbon to hydrogen atoms or the lowest whole number ratio of carbon atoms to hydrogen atoms?
4.  According to Model 1, is the empirical formula for a compound always different from the molecular formula of a compound? If no, describe a case when these two formulas would be the same.

5. Imagine you are helping a friend who missed class today. Briefly explain to your friend how to write the empirical formula for a compound when given the molecular formula.
6. Could a specific compound be identified uniquely by its empirical formula? Justify your answer with specific examples from Model 1.
7. Write the empirical formulas for each of the following compounds.



Model 2 – Percent Composition

Compound Name	Molecular Formula	Moles Carbon in 1 Mole of Compound	Moles Hydrogen in 1 Mole of Compound	Grams Carbon in 1 Mole of Compound	Grams Hydrogen in 1 Mole of Compound	Carbon % Mass	Hydrogen % Mass
Methane	CH ₄	1.00 mole	4.00 moles	12.00 g	4.00 g	75.0%	25.0%
Ethene (ethylene)	C ₂ H ₄	2.00 moles	4.00 moles	24.00 g	4.00 g	85.7%	14.3%
Propene	C ₃ H ₆	3.00 moles	6.00 moles	36.00 g	6.00 g	85.7%	14.3%
Ethyne (acetylene)	C ₂ H ₂						
Benzene	C ₆ H ₆						
1,3-butadiene	C ₄ H ₆						
Propane	C ₃ H ₈						

8. Consider the data in Model 2. Discuss as a group how the values were obtained in each column, then divide the work for completing the remaining four compounds. Show your work below.

9. Refer to Model 2. What do you notice about the percent composition of compounds with the same empirical formulas?



10. Could a specific compound be identified uniquely by its percent composition? Justify your answer with specific examples from Model 2.



11. Use the data in Model 2 to perform the following calculations by first discussing as a group how the calculations would be done, and then dividing the work among group members. List your answers in the table below. Several of the calculations have been done for you as examples.
- Calculate the lowest whole number ratio of moles of carbon in 1 mole of compound to moles of hydrogen in 1 mole of compound.
 - Calculate the lowest whole number ratio of mass of carbon in 1 mole of compound to mass of hydrogen atoms in 1 mole of compound.
 - Calculate the lowest whole number ratio of carbon percent mass to hydrogen percent mass for each compound. *Hint:* If the lowest whole number ratio is not clear by inspection, divide both values by the lesser of the two numbers.

Molecular Formula	Empirical Formula	Lowest Ratio of Moles C : Moles H	Lowest Ratio of Mass C : Mass H	Lowest Ratio of % C : % H
CH ₄	CH ₄	1 : 4	3 : 1	3 : 1
C ₂ H ₄	CH ₂	1 : 2	6 : 1	6 : 1
C ₃ H ₆	CH ₂	1 : 2	6 : 1	6 : 1
C ₂ H ₂				
C ₆ H ₆				
C ₄ H ₆				
C ₃ H ₈				

- Which of the ratios in the table above correlates best to the empirical formula of the compound?
12. Compare the ratio of mass carbon to mass hydrogen to the ratio of percent mass carbon to percent mass hydrogen for any compound in Model 2 (the table in Question 11 might be helpful as well). Do they match?

Read This!

When chemists are working with a new or unknown compound, one method they can use to determine the chemical formula of the substance is to determine the percent composition. There are several methods for chemically breaking down a compound and finding the relative masses of the elements in the substance. These data are then used to determine the empirical formula of the substance. Although this does not provide the molecular formula, it is a step in the right direction.

13. Consider the four samples of methane below. According to Model 2, the percent composition for methane is 75.0% carbon and 25.0% hydrogen. Use this information to fill in the table below. Divide the work among group members. Show your work for each calculation.

Total Mass of Methane Sample	100.0 g	72.0 g	12.0 g	10.0 g
Grams of Carbon Atoms				
Moles of Carbon Atoms				
Grams of Hydrogen Atoms				
Moles of Hydrogen Atoms				
Lowest Whole Number Ratio of Moles C : Moles H				

14. Refer to your work in Question 13.
- Can the empirical formula of a compound be derived mathematically from percent composition data? Justify your answer.
 - Would you need to know the mass of the sample when determining a compound's empirical formula from percent composition data?



15. List the steps needed to find the empirical formula for a compound when given the percent composition.
16. An unknown compound contains 50% sulfur and 50% oxygen. Determine the empirical formula of the compound. Show mathematical calculations to support your answer.
17. Explain why the empirical formula of the compound in Question 16 is not SO even though its percent composition is 50:50.



18. An unknown compound contains 43.6% phosphorus and 56.4% oxygen. Determine the empirical formula of the compound. Show mathematical calculations to support your answer.

19. Do you know the molecular formula of either of the compounds in Questions 16 or 18? Explain your reasoning.

Read This!

The empirical formula of an unknown compound can be derived from percent composition data, but you still will not know which compound you have. You will, however, have narrowed down the possibilities. For example, if you know the empirical formula of a compound is C_2H_3 , the molecular formula might be C_2H_3 , C_4H_6 , C_6H_9 , C_8H_{12} , etc. In order to determine the molecular formula of a compound, you must know the compound's molar mass. This will allow you to determine which multiple of the empirical formula is the correct molecular formula.

-  20. The molar mass of the compound in Question 18 is 283.88 g/mole. Use complete sentences to explain how this information could be used to determine the molecular formula of the compound. *Hint:* This question is not asking you to simply determine the molecular formula.



21. Nicotine is a stimulant found in the tobacco plant. The percent composition is: 74.03% C, 8.70% H and 17.27% N.
- a. Determine the empirical formula of nicotine.

- b. The molar mass of nicotine is 163.23 g/mole. Using this information and your answer to part a, calculate the molecular formula of nicotine.

Extension Questions

Model 3 – Isomers

Structural Formula	Molecular Formula	Empirical Formula
1-hexene $\text{CH}_3\text{—CH}_2\text{—CH}_2\text{—CH}_2\text{—CH=CH}_2$		
3,3-dimethyl-1-butene $\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3\text{—C—CH=CH}_2 \\ \\ \text{CH}_3 \end{array}$		
cyclohexane $\begin{array}{ccc} & \text{CH}_2\text{—CH}_2 & \\ & / \quad \backslash & \\ \text{CH}_2 & & \text{CH}_2 \\ & \backslash \quad / & \\ & \text{CH}_2\text{—CH}_2 & \end{array}$		

22. Determine the molecular formula and empirical formula for each of the compounds in Model 3.
23. In all cases, can a specific compound be identified uniquely by its molecular formula? Justify your answer with specific examples from Model 3.
-  24. The three substances in Model 3 are isomers. Write a definition for the term isomers.
25. What are the advantages and disadvantages of using structural formulas to represent a compound?
26. Make a prediction. Do you think the isomers in Model 3 will have the same physical properties such as melting point, boiling point and solubility? Explain your reasoning.

27. Make a prediction. Do you think the isomers in Model 3 will have the same chemical properties? Explain your reasoning.
28. Find the three compounds in Model 3 in a textbook or on the Internet. Compare their physical and chemical properties. Are the three compounds really just the same substance or are they different substances? Justify your answer with information you find in your research.