Determining the Empirical Formula of A Hydrated Compound

Introduction

The empirical formula of a compound is defined as the "simplest whole number ratio of the atoms" in a compound [1].

The best way to learn how to determine the empirical formula of a compound is to see the mechanics involved with the arithmetic manipulation of data:

E.g. 1: A compound contains 92.3% carbon and 7.7% hydrogen. Calculate the empirical formula of the compound.

To solve this problem, there are four steps:

1) "Convert" % to grams.

2) Determine the number of moles of each atom in the sample.

3) Divide both numbers of moles by the smallest number of moles (this step reduces the numbers to usable amounts).

4) Write the empirical formula.

Step 1: 92.3 g + 7.7 g = 100 g sample

Step 2:

$$92.3gC*\frac{1mol}{12gC} = 7.69mol \approx 7.7mol$$
$$7.7gH*\frac{1mol}{1gH} = 7.7mol$$

Step 3:

For C:
$$\frac{7.7}{7.7} = 1$$

For H: $\frac{7.7}{7.7} = 1$

Step 4: C_1H_1 or simply CH.

Had we been told that the molecular weight was 26 g/mol, we'd have divided 26 by 13 to see that there would have been 2 "CH" units. In other words, divide the molecular weight by the "empirical" weight and this will give you the number of empirical units in the molecular formula. The molecular formula, then, would be C_2H_2 .

The same approach is useful for the determination of the number of moles of water of hydration (crystallization) in various salts. The same steps are followed:

Example 2: A sample of CuSO₄• xH₂O on heating yielded 63.93% CuSO₄ and 36.07% H₂O. Determine the value for "x".

Step 1: 63.93 g + 36.07 g = 100 g sample

Step 2:

$$63.93 g CuSO_4 * \frac{1 mol CuSO_4}{159.5 g} = 0.4095 mol CuSO_4$$
$$36.07 g H_2O * \frac{1 mol H_2O}{18 g H_2O} = 2.00 mol H_2O$$

Step 3:

$$\frac{0.4095}{0.4095} = 1 \therefore 1 CuSO_4$$
$$\frac{2.00}{0.4095} = 4.88 \approx 5 \therefore 5 H_2O$$

Step 4: CuSO₄• $5H_2O$ or copper sulfate pentahydrate.

Experimental and Data

Supplies

Striker	Crucible tongs	Petri "boats"
Unknown hydrate of CuSO4	2-Crucible and cover	Ring stand
Clay triangle	Bunsen burner and tubing	Ring

Experiment

Obtain 2-2 gram samples of a hydrate of copper sulfate and 2 crucibles. Record the masses in the data table, below. Pay careful attention to what goes where on it.

Heat the samples in their respective crucibles in the apparatus illustrated at right.

Heat the samples for 10-15 minutes with a hot flame. After 10-15 minutes, turn off the flame, cover the crucibles with their covers and let cool to room temperature. Determine the mass of each crucible (carry to balances with the crucible tongs -- NOT your fingers) with its cover on and with the sample in the crucible and record your data in the data table below. Using this information, determine what the empirical formula for the hydrate is MW CuSO₄ = 159.55; MW for H₂O = 18).



	TRIAL 1	TRIAL 2
Mass of CuSO ₄ • xH ₂ O and crucible and cover (BEFORE heating) (g)		
Mass of crucible and cover (g)		
Mass of CuSO ₄ • xH ₂ O (BEFORE heating) (g)		
Mass of CuSO ₄ and crucible and cover (AFTER heating) (g)		
Mass of CuSO ₄ (AFTER heating) (g)		
Mass of H ₂ O (AFTER heating) (g)		
% CuSO ₄		
# mol CuSO4		
% H ₂ O		
# mol H ₂ O		
Reduced mol CuSO ₄		
AVG reduced mol CuSO ₄		Mol
Reduced mol H ₂ O		
AVG reduced mol H ₂ O		Mol
Empirical formula (fill in the blank)	CuSO ₄ •H ₂ O	

[1] Drago, R.S.: **Principles of Chemistry with Practical Perspectives** (Allen and Bacon: Boston) © 1974, p. 37, 66.