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:

$$92.3\,g\,C * \frac{1\,mol}{12\,g\,C} = 7.69\,mol \approx 7.7\,mol$$

$$7.7\,g\,H * \frac{1\,mol}{1\,g\,H} = 7.7\,mol$$

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 $CuSO_4 \bullet xH_2O$ on heating yielded 63.93% $CuSO_4$ and 36.07% H_2O. 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:

$$\frac{0.4095}{0.4095} = 1. \therefore 1\,CuSO_4$$

$$\frac{2.00}{0.4095} = 4.88 \approx 5. \therefore 5\,CuSO_4$$

Step 4: $CuSO_4 \bullet \underline{5}H_2O$ or copper sulfate pentahydrate.

Experimental and Data

Supplies

Striker	Crucible tongs	Petri "boats"
Unknown hydrate of $CuSO_4$	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 and 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 $CuSO_4$ = 159.55; MW for H_2O = 18).

	TRIAL 1	TRIAL 2
Mass of $CuSO_4 \bullet xH_2O$ and crucible and cover (BEFORE heating) (g)		
Mass of crucible and cover (g)		
Mass of $CuSO_4 \bullet xH_2O$ (BEFORE heating) (g)		
Mass of $CuSO_4$ and crucible and cover (AFTER heating) (g)		
Mass of $CuSO_4$ (AFTER heating) (g)		
Mass of H_2O (AFTER heating) (g)		
% $CuSO_4$		
# mol $CuSO_4$		
% H_2O		
# mol H_2O		
Reduced mol $CuSO_4$		
AVG reduced mol $CuSO_4$	Mol	
Reduced mol H_2O		
AVG reduced mol H_2O	Mol	
Empirical formula (fill in the blank)	$CuSO_4 \bullet$ _____H_2O	

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

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