

Experiment 4

Determination of a Chemical Formula

When atoms of one element combine with those of another, the combining ratio is typically an integer or a simple fraction; 1:2, 1:1, 2:1, and 2:3 are ratios one might encounter. The simplest formula of a compound expresses that atom ratio. Some substances with the ratios we listed include CaCl_2 , KBr , Ag_2O , and Fe_2O_3 . When more than two elements are present in a compound, the formula still indicates the atom ratio. Thus the substance with the formula Na_2SO_4 indicates that the sodium, sulfur, and oxygen atoms occur in that compound in the ratio 2:1:4. Many compounds have more complex formulas than those we have noted, but the same principles apply.

To find the formula of a compound we need to find the mass of each of the elements in a weighed sample of that compound. For example, if we resolved a sample of the compound NaOH weighing 40 grams into its elements, we would find that we obtained just about 23 grams of sodium, 16 grams of oxygen, and 1 gram of hydrogen. Since the atomic mass scale tells us that sodium atoms have a relative mass of 23, oxygen atoms a relative mass of 16, and hydrogen atoms a relative mass of just about 1, we would conclude that the sample of NaOH contained equal numbers of Na, O, and H atoms. Since that is the case, the atom ratio Na:O:H is 1:1:1, and so the simplest formula is NaOH . In terms of moles, we can say that that one mole of NaOH , 40 grams, contains one mole of Na, 23 grams, one mole of O, 16 grams, and one mole of H, 1 gram, where we define the molar mass to be that mass in grams equal numerically to the sum of the atomic masses in an element or a compound. From this kind of argument we can conclude that the atom ratio in a compound is equal to the mole ratio. We get the mole ratio from chemical analysis, and from that the formula of the compound.

In this experiment we will use these principles to find the formula of the compound with the general formula $\text{Cu}_x\text{Cl}_y \cdot z\text{H}_2\text{O}$, where the x , y , and z are integers which, when known, establish the formula of the compound. (In expressing the formula of a compound like this one, where water molecules remain intact within the compound, we retain the formula of H_2O in the formula of the compound.)

The compound we will study, which is called copper chloride hydrate, turns out to be ideal for one's first venture into formula determination. It is stable, can be obtained in pure form, has a characteristic blue-green color which changes as the compound is changed chemically, and is relatively easy to decompose into the elements and water. In the experiment we will first drive out the water, which is called the water of hydration, from an accurately weighed sample of the compound. This occurs if we gently heat the sample to a little over 100°C . As the water is driven out, the color of the sample changes from blue-green to a tan-brown color similar to that of tobacco. The compound formed is anhydrous ("no water") copper chloride. If we subtract its mass from that of the hydrate, we can determine the mass of the water that was driven off, and, using the molar mass of water, find the number of moles of H_2O that were in the sample.

In the next step we need to find either the mass of copper or the mass of chlorine in the anhydrous sample we have prepared. It turns out to be much easier to determine the mass of the copper, and find the mass of chlorine by difference. We do this by dissolving the anhydrous sample in water, which gives us a green solution containing copper and chloride ions. To that solution we add some aluminum metal wire. Aluminum is what we call an active metal; in contact with a solution containing copper ions, the aluminum metal will react chemically with those ions, converting them to copper metal. The aluminum is said to reduce the copper ions to the metal, and is itself oxidized. The copper metal appears on the wire as the reaction proceeds, and has its typical red-orange color. When the reaction is complete, we remove the excess Al, separate the copper from the solution, and weigh the dried metal. From its mass we can calculate the number of moles of copper in the sample. We find the mass of chlorine by subtracting the mass of copper from that of the anhydrous copper chloride, and from that value determine the number of moles of chlorine. The mole ratio for $\text{Cu}:\text{Cl}:\text{H}_2\text{O}$ gives us the formula of the compound.

Hypothesis Of Determination Of A Chemical Formula

Аркадий Серков, Антон Серков



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systems dramatically reduce the time associated with structure elucidation and improve the reliability of the results Contemporary Computer Assisted Approaches to Molecular Structure Elucidation describes the principles on which these expert systems for spectroscopic structure elucidation are based and concisely explains the algorithmic concepts behind the programs The authors use their own personal experiences in the development of the Structure Elucidator StrucEluc CASE software system to discuss the present state of the art in computer assisted structure elucidation Scientists that are presently using CASE systems will be interested in the algorithms and modern approaches and for organizations that are currently using the StrucEluc platform the book is designed to help researchers understand the strategies behind CASE as well as details regarding the StrucEluc platform For scientists that have never used CASE systems they will now have access to all necessary information to understand CASE systems for mastering this new and very effective approach to structure elucidation The authors overall goal is writing this book is to produce the must read definitive text that will represent the results of decades of work to develop computer assisted structure elucidation software systems CASE systems are now powerful software tools commonly outperforming and correcting human interpretations of data This book will also provide an historical perspective of the work of the founding fathers of the technique and identify the challenges that have been overcome to produce modern CASE systems

Computer-Based Structure Elucidation from Spectral Data Mikhail E. Elyashberg, Antony J. Williams, 2015-02-27 Here the authors introduce readers to solving molecular structure elucidation problems using the expert system ACD Structure Elucidator They explain in detail the concepts of the Computer Assisted Structure Elucidation CASE approach and point out the crucial role of understanding the axiomatic nature of the data used to deduce the structure Aspects covered include the main blocks of the expert system and essential features of the mathematical algorithms used Graduate and PhD students as well as practicing chemists are provided with a detailed explanation of the various practical approaches depending on available spectral data peculiarities and the complexity of the unknown structure This is supported by a large number of real world completed examples most of which are related to the structure elucidation of natural product molecules containing unusual skeletons Dedicated software and further supplementary material are available at www.acdlabs.com TeachingSE

Confidential Documents United States. Army Air Forces, 1942

Outlines of Physical Chemistry George Senter, 1915

Fungal Biology R. K. Sharma, Vijay Kumar, 2007

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