Chemists use the elemental composition of compounds to determine their formulas (and vice-versa). We'll look at some of the hyperbole surrounding salt and salt additives to explore the meaning of formulas.

Here are a few of the claims by salt manufacturers that we can examine scientifically:

• "sea salt" is better nutritionally than "regular salt"
• salt additives are harmful
• "kosher salt" tastes better than regular table salt.
• "exotic salts" are more flavorful (see the figures).
• freshly ground salt is superior

Nutrition

FDA requires that food grade salt be at least 97.5% NaCl, but it's usually much purer. Sea salt is usually about 99% NaCl, because it is the salt in highest concentration, and precipitates first in nearly pure form when sea water is condensed. Sea salt is not a significant source of any nutrients except NaCl. We can tell from the formula that salt must be 39.34% Na and 60.66% Cl (see below), so there can be little debate about one kind of salt being different or "better" than another, except if there are significant amounts of additives.

Additives
Iodine

Some "sea salts" have no additives, but most salt contains potassium iodide (KI) or cuprous iodide (CuI) as additives which provide the essential mineral nutrient iodine. This additive prevents thyroid disease. We'll see below that the additive with the least iodine per gram is often used, and explain why.

Reducing Sugars

If KI is added to the salt, an additional additive must be added to protect it from oxidation by air to give elemental iodine (I$_2$), which has no nutritive value (and is actually toxic). One reducing sugar is explored below in an example.

Anti-caking agents

Salts also contain anti-caking agents to prevent them from clumping in damp air, but those additives are usually insoluble and innocuous, and present at very low levels. Morton's table salt contains 0.2 to 0.7% calcium silicate, which explains why solutions of table salt are cloudy. Morton's Coarse Kosher Salt contains sodium ferrocyanide [Na$_4$Fe(CN)$_6$] as an anticaking agent, which can decompose in acid to give cyanide, but the concentration is 0.0013%, so low that it can't be a problem.

Kosher Salt

Kosher salt is made for coating raw meat or poultry to purify it, so its crystals are irregular and large which may create "bursts of saltiness" superior to regular table salt when used to salt food. This is the only reason why freshly ground salt is superior (it has no aroma to release as freshly ground pepper does).

Exotic Salts

Boutique salts from around the world may be gray to black, pinkish to red, or other hues, and do have different flavors due to the impurities they contain.

The Usefulness of Formulas

We have presented a microscopic view of the chemical reaction between potassium (a reactive metal) and iodine (a poisonous purple solid) to form white, nutritious KI. The equation

\[
\ce{K(s) + I2(s) → KI(s)} \quad \text{Label[1]}
\]

represent the same event in terms of chemical symbols and formulas.

We also noted that the reaction between Cu and I$_2$, or between Cu$^{2+}$ and I$^-$ gives CuI, not CuI$_2$:

\[
\ce{2 Cu^{2+} + 4 I^- → 2 Cu + I2} \quad \text{Label[2]}
\]
But how does a practicing chemist find out what is occurring on the microscopic scale? In the case of reaction (2) above, we would expect CuI\textsubscript{2} so how do we know the product is CuI?

When a reaction is carried out for the first time, little is known about the microscopic nature of the products. It is therefore necessary to determine experimentally the composition and formula of a newly synthesized substance.

The first step in such a procedure is usually to separate and purify the products of a reaction. The low solubility of CuI in water would permit purification by recrystallization. The product could be dissolved in a small quantity of hot water and filtered to remove undissolved impurities. Upon cooling and partial evaporation of the water, crystals of relatively pure CuI would form. Comparing its properties, like color and melting point, with a handbook or table of data leads to the conclusion that it is CuI.

But suppose you were the first person who ever prepared CuI. There were no tables which listed its properties then, and so how could you determine that the formula should be CuI? One answer involves quantitative analysis—the determination of the percentage by mass of each element in the compound. Such data are usually reported as the percent composition.

Example 

When 10.0 g copper reacts with sufficient iodine, 29.97 g of a pure compound is formed. Calculate the percent composition from these experimental data.

Solution

The percentage of mercury is the mass of mercury divided by the total mass of compound times 100 percent:

The remainder of the compound (29.97 g – 10 g = 19.97 g) is iodine:

As a check, verify that the percentages add to 100: 66.6% + 33.4% = 100%

Calculating Formulas from % Composition

To obtain the formula from percent-composition data, we must find how many iodine atoms there are per copper atom. On a macroscopic scale this corresponds to the ratio of the amount of iodine to the amount of copper. If the formula is CuI, it not only indicates that there is one iodine atom per copper atom, it also says that there is 1 mol of iodine atoms for each 1 mol of copper atoms. That is, the amount of iodine is the same as the amount of copper. The numbers in the ratio of the amount of iodine to the amount of copper (1:1) are the subscripts of iodine and copper in the formula, although when they are 1, the subscripts are omitted (Cu\textsubscript{1}I\textsubscript{1} = CuI).

EXAMPLE 2 Determine the formula for the compound whose percent composition was calculated in the previous example.

Solution For convenience, assume that we have 100 g of the compound. Of this, 66.6 g (66.6%) is iodine and 33.4 g is copper. Each mass can be converted to an amount of substance

Dividing the larger amount by the smaller, we have
The ratio 1.03 mol Cu to 1 mol I also implies that there is 1.03 Cu atom per 1 I atom. If the atomic theory is correct, there is no such thing as 0.03 Cu atom; furthermore, our numbers are only good to three significant figures. Therefore we round 1.03 to 1 and write the formula as CuI.

**EXAMPLE 3** An unstable iodide of copper is isolated at low temperature and is found to have the composition 20.0% Cu, 80.0% I. Find its formula.

**Solution** Again assume a 100-g sample and calculate the amount of each element:

The ratio is

We would therefore assign the formula CuI$_2$.

The formula determined by this method is called the **empirical formula** or **simplest formula**. Occasionally, the empirical formula differs from the actual molecular composition, or the **molecular formula**, because the ratio 1:2 is the same as 2:4. For example, a compound of N and O with the empirical formula NO$_2$ may actually be N$_2$O$_4$. Experimental determination of the molecular weight in addition to percent composition permits calculation of the molecular formula.

**Reducing Sugars**

If KI is added to salt, a "reducing sugar" is added to protect the KI from oxidation by air to give iodine (which is violet, but vaporizes easily and is lost by the salt), especially in the presence of moisture and acid, which supplies H$^+$:

$$4 \text{H}^+ + 4 \text{KI} + \text{O}_2 \rightarrow 2 \text{H}_2\text{O} + \text{I}_2$$

The reducing sugar reacts with the oxygen (or other oxidizing agents which may be present) before this reaction can occur.

**EXAMPLE 4** An antioxidant in Morton’s table salt is found to have a composition of 40.00% C, 53.28% O, and 6.713% H, and its molecular weight is 180.16 by freezing point depression measurements. Determine its empirical and molecular formulas.

**Solution**

Dividing each by the smallest:

Dividing each by the smallest:

The empirical formula is therefore CH$_2$O. The molecular weight corresponding to the empirical formula is

$$12.01 + 2 \times 1.008 + 15.9994 = 30.03$$

Since the experimental molecular weight is 180.16, this represents 180.16/30.03 or 6.0 x as great, all subscripts must be multiplied by 6, and the molecular formula is C$_6$H$_{12}$O$_6$. Dextrose is a reducing sugar, due to the C=O group of the open chain structure.
Occasionally the ratio of amounts is not a whole number.

Anticaking Agents

A common anticaking agent is calcium silicate, CaSiO$_3$, but zeolites and calcium minerals like "bone ash" are commonly used.

**EXAMPLE 5** A sample of "bone ash" anticaking agent contains 38.76% Ca, 19.971% P, and 41.26% O. What is its empirical formula?

**Solution**

Divide all three by the smallest amount of substance

Clearly there are four times as many O atoms as P atoms, but the ratio of Ca to P is less obvious. We must convert 1.5 to a ratio of small whole numbers. This can be done by changing the figures after the decimal point to a fraction. In this case, .5 becomes 1/2. Thus 1.5 = 2/2 + 1/2 =

. [in a more complicated case, like 2.25, .25 becomes ¼. Thus 2.25 = 2¼ =

].

We can also write

Thus the empirical formula is Ca$_3$P$_2$O$_8$, which is tricalcium phosphate (Ca$_3$(PO$_4$)$_2$), an important nutritional supplement and mineral.

Calculating Percent Composition of NaCl, KI, and CuI from Formulas

Once someone has determined a formula—empirical or molecular—it is possible for someone else to do the reverse calculation. Finding the weight-percent composition from the formula often proves quite informative, as the following example shows.

**EXAMPLE 6**

a. Prove that all NaCl is 39.34% Na and 60.66% Cl, as claimed above.

b. Which of the nutritional supplements, KI or CuI, has the highest percent I?

**Solution**

a. 1 mol NaCl contains 1 mol Na and 1 mol Cl. The molar mass is thus

\[ M = 22.99 + 35.45 = 58.44 \text{ g mol}^{-1} \]

A 1-mol sample of NaCl would weigh 58.44 g. The mass of 1 mol Na it contains is
Therefore the percentage of Na is

The percentage of Cl must be 100% - 39.34% = 60.66%, but we can check:

Therefore the percentage of Cl is

b.

1 mol KI contains 1 mol K and 1 mol I. The molar mass is thus

\[ M = 39.098 + 126.9 = 166.0 \text{ g mol}^{-1} \]

Similarly, the molar mass of CuI is 190.45.

A 1-mol sample of KI would weigh 166.0 g. The mass of 1 mol I it contains is

Therefore the percentage of I is

The percentage of K must be 100% - 76.5% = 23.5%, but we can check:

Therefore the percentage of K is

The percentages of I in CuI is

Even though CuI has a smaller %I, (KI provides more I per gram), it is often used because it is less subject to the oxidation of the iodide than KI.

References

1. ↑ en.Wikipedia.org/wiki/Black_lava_salt
2. ↑ en.Wikipedia.org/wiki/Kala_Namak

Contributors and Attributions

- Ed Vitz (Kutztown University), John W. Moore (UW-Madison), Justin Shorb (Hope College), Xavier Prat-Resina (University of Minnesota Rochester), Tim Wendorff, and Adam Hahn.