Writing Ionic Formulas

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Printed: November 25, 2013

CONCEPT 1

Writing Ionic Formulas

Lesson Objectives

The student will:

- provide the correct formulas for binary ionic compounds.
- provide the correct formulas for compounds containing metals with variable oxidation numbers.
- provide the correct formulas for compounds containing polyatomic ions.

Vocabulary

- empirical formula
- formula unit

Introduction

Ionic compounds do not exist as molecules. In the solid state, ionic compounds are in crystal lattices containing many cations and anions. An ionic formula, like NaCl, is an empirical formula. The **empirical formula** gives the simplest whole number ratio of atoms of each element present in the compound. The formula for sodium chloride merely indicates that it is made of an equal number of sodium and chloride ions. As a result, it is technically incorrect to refer to a molecule of sodium chloride. Instead, one unit of NaCl is called the **formula unit**. A formula unit is one unit of an empirical formula for an ionic compound.

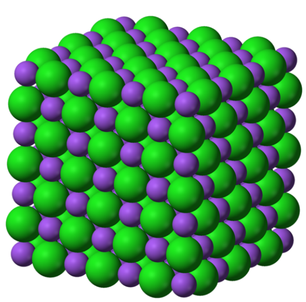


FIGURE 1.1
The three-dimensional crystal lattice structure of sodium chloride.

Sodium sulfide, another ionic compound, has the formula Na_2S. This formula indicates that this compound is made up of twice as many sodium ions as sulfide ions. Na_2S will also form a crystal lattice, but the lattice won't be the same as the NaCl lattice because the Na_2S lattice has to have two sodium ions per sulfide ion.

Predicting Formulas for Ionic Compounds

Determining Ionic Charge

The charge that will be on an ion can be predicted for most of the monatomic ions. Many of these ionic charges can be predicted for entire families of elements. There are a few ions whose charge must simply be memorized, and there are also a few that have the ability to form two or more ions with different charges. In these cases, the exact charge on the ion can only be determined by analyzing the ionic formula of the compound.

All of the elements in family 1A are metals that have the same outer energy level electron configuration, the same number of valence electrons (one), and low first ionization energies. Therefore, these atoms will lose their one valence electron and form ions with a $+1$ charge. This allows us to predict the ionic charges on all the 1A ions: Li^+, Na^+, K^+, Rb^+, Cs^+, and Fr^+.

Hydrogen is a special case. It has the ability to form a positive ion by losing its single valence electron, just as the 1A metals do. In those cases, hydrogen forms the $+1$ ion, H^+. In rare cases, hydrogen can also take on one electron to complete its outer energy level. These compounds, such as NaH, KH, and LiH, are called hydrides. Hydrogen also has the ability to form compounds without losing or gaining electrons, which will be discussed in more details in the chapter "Covalent Bonds and Formulas."

All of the elements in family 2A have the same outer energy level electron configuration and the same number of valence electrons (two). Each of these atoms is a metal with low first and second ionization energies. Therefore, these elements will lose both of its valence electrons to form an ion with a $+2$ charge. The ions formed in family 2A are: Be^{2+}, Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, and Ra^{2+}.

There is a slight variation for the elements in family 3A. The line separating metals from nonmetals on the periodic table cuts through family 3A between boron and aluminum. In family 3A, boron, $1s^22s^22p^1$, behaves as a nonmetal due to its higher ionization energy and higher electron affinity. Aluminum, on the other hand, is on the metallic side of the line and behaves as an electron donor. Aluminum, $1s^22s^22p^63s^23p^1$, always loses all three of its valence electrons and forms an Al^{3+} ion. Gallium and indium have the same outer energy level configuration as aluminum, and they also lose all three of their valence electrons to form the $+3$ ions Ga^{3+} and In^{3+}. Thallium, whose electron configuration ends with $6s^26p^1$, could also form a $+3$ ion, but for reasons beyond the scope of this book, thallium is more stable as the $+1$ ion Tl^+.

All the elements in the 6A family have six valence electrons, and they all have high electron affinities. These atoms will, therefore, take on additional electrons to complete the octet of electrons in their outer energy levels. Since each atom will take on two electrons to complete its octet, members of the 6A family will form -2 ions. The ions formed will be: O^{2-}, S^{2-}, Se^{2-}, and Te^{2-}.

Family 7A elements have the outer energy level electron configuration ns^2np^5. These atoms have the highest electron affinities in their periods and will each take on one more electron to complete the octet of electrons in the outer energy levels. Therefore, these atoms will form -1 ions: F^-, Cl^-, Br^-, I^-, and At^-.

Family 8A elements have completely filled outer energy levels. Because of this, it is very energetically unfavorable to either add or remove electrons, and elements found in family 8A do not form ions.

Transition Elements

There are greater variations in the charge found on ions formed from transition elements. Many of the transition elements can form ions with different charges. We will consider some of these elements later in this chapter. There are also some transition elements that only form one ion.

Consider the electron configuration of silver, Ag, is $1s^22s^22p^63s^23p^64s^23d^{10}4p^65s^14d^{10}$. When forming an ion, silver loses its single valence electron to produce Ag^+. Note that its electron configuration does not exactly follow the rules that you have been shown for filling orbitals. Electrons have been placed in 4 d orbitals even though the 5s orbital, which is usually lower in energy, is not completely full. Because the 4d and 5s orbitals are so similar in energy, very small perturbations can sometimes make it energetically favorable for the 5s electron to move into a 4d orbital. It happens that a set of half full (5 electrons) or completely full (10 electrons) d orbitals gives a little extra stability to the electron configuration. This also happens with chromium, copper, molybdenum, and gold.

The electron configuration for Zn is $[Ar]4s^2 3d^{10}$. Like main group metals, zinc loses all of its valence electrons when it forms an ion, so it forms a Zn^{2+} ion. Cadmium is similar. The electron configuration for Cd is $[Kr]5s^2 3d^{10}$, so it forms a Cd^{2+} ion.

Writing Basic Ionic Formulas

In writing formulas for binary ionic compounds (binary refers to two elements, *not* two single atoms), the cation is always written first. Chemists use subscripts following the symbol of each element to indicate the number of that element present in the formula. For example, the formula Na_2O indicates that the compound contains two atoms of sodium for every one oxygen. When the subscript for an element is 1, the subscript is omitted. The number of atoms of an element with no indicated subscript is always read as 1. When an ionic compound forms, the number of electrons given off by the cations must be exactly the same as the number of electrons taken on by the anions. Therefore, if calcium, which gives off two electrons, is to be combined with fluorine, which takes on one electron, then one calcium atom must combine with two fluorine atoms. The formula would be CaF_2.

Suppose we wish to write the formula for the compound that forms between aluminum and chlorine. To write the formula, we must first determine the oxidation numbers of the ions that would be formed. We will revisit the concept of oxidation numbers later, but for now, all you need to know is that the oxidation number for an atom in an ionic compound is equal to the charge of the ion it produces.

$$\begin{array}{cc} 3+ & 1- \\ \text{Al} & \text{Cl} \end{array}$$

Then, we determine the simplest whole numbers with which to multiply these charges so they will balance (add to zero). In this case, we would multiply the 3+ by 1 and the 1− by 3.

$$\begin{array}{cc} 3+ & 1- \\ \text{Al} & \text{Cl} \\ (3+)(1) = 3+ & (1-)(3) = 3- \end{array}$$

You should note that we could multiply the 3+ by 2 and the 1− by 6 to get 6+ and 6−, respectively. These values will also balance, but this is *not* acceptable because empirical formulas, by definition, must have the lowest whole number multipliers. Once we have the *lowest* whole number multipliers, those multipliers become the subscripts for the symbols. The formula for this compound would be $AlCl_3$.

Here's the process for writing the formula for the compound formed between aluminum and sulfur.

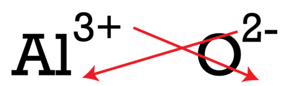
$$\begin{array}{cc} 3+ & 2- \\ \text{Al} & \text{S} \\ (3+)(2) = 6+ & (2-)(3) = 6- \end{array}$$

Therefore, the formula for this compound would be Al_2S_3.

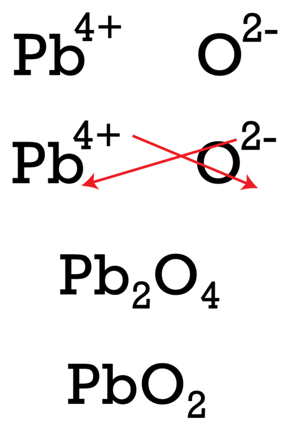
Another method used to write formulas is called the criss-cross method. It is a quick method, but it often produces errors if the user doesn't pay attention to the results. The example below demonstrates the criss-cross method for writing the formula of a compound formed from aluminum and oxygen. In the criss-cross method, the oxidation numbers are placed over the symbols for the elements just as before.

$$\overset{3+}{\text{Al}} \qquad\qquad\qquad \overset{2-}{\text{O}}$$

In this method, the oxidation numbers are then criss-crossed and used as the subscripts for the other atom (ignoring sign).



This produces the correct formula Al_2O_3 for the compound. Here's an example of a criss-cross error:



If you used the original method of finding the lowest multipliers to balance the charges, you would get the correct formula PbO_2, but the criss-cross method produces the incorrect formula Pb_2O_4. If you use the criss-cross method to generate an ionic formula, it is essential that you check to make sure that the subscripts correspond to the lowest whole number ratio of the atoms involved. Note that this only applies to ionic compounds. When we learn about covalent compounds in the chapter "Covalent Bonds and Formulas," you will see that the formula N_2O_4 describes a different molecule than NO_2, so it would not be reduced to its simplest ratio.

Metals with Variable Oxidation Number

When writing formulas, you are given the oxidation number. When we get to naming ionic compounds, however, it is absolutely vital that you are able to recognize metals that can have more than one oxidation number. A partial list of metals with variable oxidation numbers includes iron, copper, tin, lead, nickel, and gold.

For example, iron can form both Fe^{2+} and Fe^{3+} ions. The electron configuration for neutral Fe is $1s^22s^22p^63s^23p^64s^23d^6$. It is fairly straightforward as to why iron forms the 2+ ion, because it loses all of its valence electrons like other metals do. The electron configuration for the Fe^{2+} ion is $[\text{Ar}]3d^6$. Why would the iron ion lose one more electron? Earlier, we mentioned that the *d* orbitals have a slightly lower energy when they are exactly half full or completely full. If this Fe^{2+} ion were to lose one more electron, the 3*d* orbitals would be exactly half full with five electrons. When iron reacts, it will first form Fe^{2+}. However, if the pull on its electrons is particularly strong, it will form Fe^{3+}.

Other examples of metals with variable oxidation states are less intuitive. For example, copper, silver, and gold (a single family of metals) can all lose a single electron to form Cu^{+}, Ag^{+}, and Au^{+}. All subshells in the resulting ions are completely full or empty. However, copper can also form Cu^{2+}, which is actually more stable in many cases. Gold can form Au^{3+}, but Au^{2+} is rarely observed. Silver, as we mentioned earlier, does not commonly lose more than one electron.

The oxidation states available to main group metals are generally easy to predict. However, tin and lead are two exceptions. In addition to losing all four of their valence electrons to make Sn^{4+} and Pb^{4+}, tin and lead will also commonly form Sn^{2+} and Pb^{2+} ions. There are many metals with variable oxidation states, but it is worth memorizing at least the ones mentioned here (Fe, Cu, Au, Sn, Pb).

Polyatomic Ions

Polyatomic ions require additional consideration when you write formulas involving them. Recall from earlier this list of common polyatomic ions:

- Ammonium ion, NH_4^{+}
- Acetate ion, $C_2H_3O_2^{-}$
- Carbonate ion, CO_3^{2-}
- Chromate ion, CrO_4^{2-}
- Dichromate ion, $Cr_2O_7^{2-}$
- Hydroxide ion, OH^{-}
- Nitrate ion, NO_3^{-}
- Phosphate ion, PO_4^{3-}
- Sulfate ion, SO_4^{2-}
- Sulfite ion, SO_3^{2-}

Suppose we are asked to write the formula for the compound that would form between calcium and the nitrate ion. We begin by putting the charges above the symbols just as before.

$$\begin{array}{cc} 2+ & 1- \\ \text{Ca} & \text{NO}_3 \\ (2+)(1) = 2+ & (1-)(2) = 2- \end{array}$$

The multipliers needed to balance these ions are 1 for calcium and 2 for nitrate. We wish to write a formula that tells our readers that there are two nitrate ions in the formula for every calcium ion. When we put the subscript 2 beside the nitrate ion in the same fashion as before, we get something strange – $CaNO_{32}$. With this formula, we are indicating 32 oxygen atoms, which is wrong. The solution to this problem is to put parentheses around the nitrate ion before the subscript is added. Therefore, the correct formula is $Ca(NO_3)_2$. Similarly, calcium phosphate would be $Ca_3(PO_4)_2$. If a polyatomic ion does not need a subscript other than an omitted 1, then the parentheses are not needed. Although including these unnecessary parentheses does not change the meaning of the formula, it may cause the reader to wonder whether a subscript was left off by mistake. Try to avoid using parentheses when they are not needed.

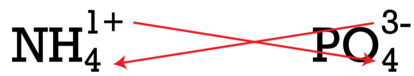
Example:

Write the formula for the compound that will form from aluminum and acetate.

The charge on an aluminum ion is $+3$, and the charge on an acetate ion is -1. Therefore, three acetate ions are required to combine with one aluminum ion. This is also apparent by the criss-cross method. However, we cannot place a subscript of 3 beside the oxygen subscript of 2 without inserting parentheses first. Therefore, the formula will be $Al(C_2H_3O_2)_3$.

Example:

Write the formula for the compound that will form from ammonium and phosphate.



The charge on an ammonium ion is $+1$ and the charge on a phosphate ion is -3. Therefore, three ammonium ions are required to combine with one phosphate ion. The criss-cross procedure will place a subscript of 3 next to the subscript 4. This can only be carried out if the ammonium ion is first placed in parentheses. Therefore, the proper formula is $(NH_4)_3PO_4$.

Example:

Write the formula for the compound that will form from aluminum and phosphate.

$$Al^{3+} \qquad PO_4{}^{3-}$$

Since the charge on an aluminum ion is $+3$ and the charge on a phosphate ion is -3, these ions will combine in a one-to-one ratio. In this case, the criss-cross method would produce an incorrect answer. Since it is not necessary to write the subscripts of 1, no parentheses are needed in this formula. Since parentheses are not needed, it is generally considered incorrect to use them. The correct formula is $AlPO_4$.

More Examples:

Magnesium hydroxide ......$Mg(OH)_2$

Sodium carbonate ....Na_2CO_3

Barium acetate ....$Ba(C_2H_3O_2)_2$

Ammonium dichromate ....$(NH_4)_2Cr_2O_7$

Lesson Summary

- The oxidation number for ions of the main group elements can usually be determined by the number of valence electrons.
- Some transition elements have fixed oxidation numbers, while others have variable oxidation numbers.
- Some metals, such as iron, copper, tin, lead, and gold, also have variable oxidation numbers.
- Formulas for ionic compounds contain the lowest whole number ratio of subscripts such that the sum of all positive charges equals the sum of all negative charges.

Further Reading / Supplemental Links

This website provides more details about ionic bonding, including a conceptual simulation of the reaction between sodium and chlorine. The website also discusses covalent bonding, the focus of the chapter "Covalent Bonds and Formulas."

- http://visionlearning/library/module_viewer.php?mid=55

Review Questions

1. Fill in the chart below (**Table** 1.1) by writing formulas for the compounds that might form between the ions in the columns and rows. Some of these compounds don't exist but you can still write formulas for them.

TABLE 1.1:

	Na^+	Ca^{2+}	Fe^{3+}	NH_4^+	Sn^{4+}
NO_3^-					
SO_4^{2-}					
Cl^-					
S^{2-}					
PO_4^{3-}					
OH^-					
$Cr_2O_7^{2-}$					
CO_3^{2-}					

References

1. Benjah-bmm27. 3D structure of sodium chloride. Public domain