CHEMICAL FORMULAS AND
FORMULA WEIGHT CALCULATIONS

1. THE MEANING OF A CHEMICAL FORMULA

A chemical formula is a shorthand method of representing the elements in a compound. The formula shows the formulas of the elements in the compound and the ratio of the elements to one another. For example, the forumla for sodium chloride:

$$NaCl$$

tells us that the compound is composed of the elements sodium, Na, and chlorine, Cl, in a one-to-one ratio. That is, one atom of sodium combines with one atom of chlorine.

When elements combine in different ratios, subscripts are added, following the element symbol, to -indicate that the number of atoms of that element in the compound if it is greater than one. The subscript refers only to the element it immediately follows. For example, the formula for magnesium bromide:

$$MgBr_2$$

tells us that two bromine atoms combine with one magnesium atom.

Some elements form stable groups, or polyatomic ions, that combine with other elements to form compounds. An example of this is the sulfate polyatomic ion in the compound calcium sulfate:

$$CaSO_4$$

In this compound, the SO_4 is called a *sulfate* group. It consists of one sulfur atom combined with four oxygen atoms. The sulfate group cannot exist by itself and must be combined with another element. The compound $CaSO_4$ consists of one calcium atom combined with one sulfate group. Counting atoms, calcium sulfate consists of one calcium atom, one sulfur atom, and four oxygen atoms.

Another example of an atom combined with a polyatomic ion is barium nitrate:

$$Ba(NO_3)_2$$

This compound consists of a barium atom combined with two nitrate groups. Since NO_3 is readily identified as a nitrate group, and barium combines with two nitrates, parentheses are placed around the nitrate and the subscript 2 indicates two nitrate groups. Changing the subscripts in the nitrate to N_2O_6 would chang e the meaning of the formula and is incorrect. Counting atoms, barium nitrate consists of one barium atom, two nitrogen atoms, and six oxygen atoms.

In the compound zinc phosphate:

$$Zn_3(PO_4)_2$$
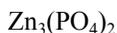
we encounter another polyatomic ion, phosphate, PO_4. In this example, three atoms of zinc combine with two phosphate groups. Counting atoms, there are three atoms of zinc, two atoms of phosphorus, and eight atoms of oxygen.

The meaning of these formulas are summarized in Figure 1.

Figure 1. The meaning of some chemical formulas.

NaCl

Symbol indicates the element sodium

Symbol indicates the element chlorine

No subscripts indicate only one atom of each element

$MgBr_2$

Symbol indicates the element magnesium

Subscript indicates two atoms of bromine

No subscript indicates only one atom of magnesium

Symbol indicates the element bromine

$CaSO_4$

Symbol indicates the element calcium

Formula indicates the sulfate polyatomic ion consisting of the elements sulfur and oxygen

No subscript indicates only one atom of calcium

Subscript indicates four atoms of oxygen in one sulfate group

No subscript indicates one atom of sulfur in one sulfate group

$Ba(NO_3)_2$

Symbol indicates the element barium

Formula indicates the nitrate polyatomic ion consisting of the elements nitrogen and oxygen

No subscript indicates only one atom of barium

Subscript indicates two nitrate polyatomic ions

No subscript indicates one atom of nitrogen in one nitrate group

Subscript indicates three atoms of oxygen in one nitrate group

Formula indicates the
phosphate polyatomic ion
consisting of the elements
phosphorus and oxygen

Symbol indicates
the element zinc

$$Zn_3(PO_4)_2$$

Subscript indicates
three atoms of zinc

Subscript indicates two
phosphate polyatomic ions

No subscript indicates
one atom of phosphorus
in one phosphate group

Subscript indicates
four atoms of oxygen
in one phosphate group

2. CALCULATING A FORMULA WEIGHT OR MOLECULAR WEIGHT

The **formula weight** of a substance (element or compound) is the sum of the atomic weights of all the atoms in the chemical formula of the substance. A **molecular weight** of a substance is the sum of all the atomic weights of all the atoms in a molecule of a molecular substance. The terms formula weight and molecular weight are often used interchangeably, but formula weight includes simple or empirical formulas of compounds, as well as, molecular formulas.

To calculate the formula weight or molecular weight of a compound, set up a table:
1. **List the elements in the compound**
2. **Determine the number of atoms of each element in the compound**
3. **Look up the atomic weight of each element and place them in the appropriate column**
4. **Multiply the number of atoms times the atomic weights to get the total mass of each element**
5. **Add the total masses of all the elements.**

Examples:

1. Calculate the formula weight of sodium chloride, NaCl.

Answer:

Set up a table listing the elements in the compound, the number of atoms of each element, and the atomic weight of each element.

Elements in the compound	Number of atoms of each element	Atomic Weight
Na	1	23.0
Cl	1	35.5

Multiply the number of atoms times the atomic weight to get the total mass of each element. Then add the total masses.

Elements in the compound	Number of atoms of each element	Atomic Weight			Total Mass
Na	1	x	23.0	=	23.0
Cl	1	x	35.5	=	35.5

Formula weight = 58.5

Although there are no units of the atomic and formula weights, the atomic weights are expressed in amu (atomic mass units) for single molecules or grams for laboratory quantities.

2. Calculate the formula weight of magnesium bromide, $MgBr_2$

Answer:

Set up a table similar to the one used in example 1.

Elements in the compound	Number of atoms of each element		Atomic Weight		Total Mass
Mg	1	x	24.3	=	24.3
Br	2	x	79.9	=	159.8
			Formula weight	=	184.1

3. Calculate the formula weight of calcium sulfate, $CaSO_4$

Answer:

Elements in the compound	Number of atoms of each element		Atomic Weight		Total Mass
Ca	1	x	40.1	=	40.1
S	1	x	32.1	=	32.1
O	4	x	16.0	=	64.0
			Formula weight	=	136.2

4. Calculate the formula weight of barium nitrate, $Ba(NO_3)_2$

Answer:

Elements in the compound	Number of atoms of each element		Atomic Weight		Total Mass
Ba	1	x	137.3	=	137.3
N	2	x	14.0	=	28.0
O	6	x	16.0	=	96.0
			Formula weight	=	261.3

5. Calculate the formula weight of zinc phosphate, $Zn_3(PO_4)_2$

Answer:

Elements in the compound	Number of atoms of each element		Atomic Weight		Total Mass
Zn	3	x	65.4	=	196.2
P	2	x	31.0	=	62.0
O	8	x	16.0	=	128.0
			Formula weight	=	386.2

Problems: Calculating formula weights

Calculate the formula weights of the following compounds.

a) $K_2S_2O_4$

b) Al_2S_3

c) Ag_2CO_3

d) $Ca(C_2H_3O_2)_2$

e) $Cr_2(SO_4)_3$

f) H_3PO_4

g) $Sn(OH)_2$

h) $Ni_2Fe(CN)_6$

i) $Mg(IO_3)_2$

j) $Co(ClO_4)_2$
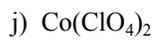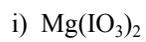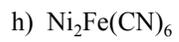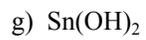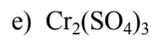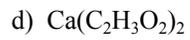
In the previous section the formula weights of NaCl, $MgBr_2$, $CaSO_4$, $Ba(NO_3)_2$ and $Zn_3(PO_4)_2$ were calculated. You will notice, however, that there were no units included with the calculated formula weights. So, what units should we use?

If we are talking about these compounds as individual molecules, then the weights or masses would be expressed in amu's (atomic mass units). But, we do not work with individual atoms or molecules, we work with amounts we can handle and measure in a laboratory setting. So, in a laboratory setting, we use gram quantities. Thus, we can call the weights (or masses) we calculated *gram* **MOLEcular weights**. A convenient short name for this is a **MOLE** (abbreviated **mol**). The proper units are **g/mol**

Compound	Gram molecular weight
NaCl	58.5 g/mol
$MgBr_2$	184.1 g/mol
$CaSO_4$	136.2 g/mol
$Ba(NO_3)_2$	261.3 g/mol
$Zn_3(PO_4)_2$	386.2 g/mol

3. Converting from grams to moles and moles to grams

To convert from grams to moles, divide the given mass by the molecular weight:

Sample problem:

How many moles are there in 50.0 g of $MgBr_2$?

Solution:

The first step is to calculate the gram molecular weight of $MgBr_2$. Since we did that previously in this exercise, we will use the value of 184.1 g/mol.

Next, set up the problem using dimensional analysis.

The conversion factor is: 1 mole $MgBr_2$ = 184.1 g $MgBr_2$

$$? \text{ moles } MgBr_2 = 50.0 \text{ g } MgBr_2 \times \frac{1 \text{ mole } MgBr_2}{184.1 \text{ g } MgBr_2}$$

$$= 0.271 \text{ mole } MgBr_2$$

To convert from moles to grams, multiply the given mass by the molecular weight:

Sample problem:

How many grams are there in 1.60 moles of $CaSO_4$?

Solution:

The first step is to calculate the gram molecular weight of $CaSO_4$. Since we did that previously in this exercise, we will use the value of 136.2 g/mol.

Next, set up the problem using dimensional analysis.

The conversion factor is: 1 mole $CaSO_4$ = 136.2 g $MgBr_2$

$$? \text{ g } CaSO_4 = 1.60 \text{ mole } CaSO_4 \times \frac{136.2 \text{ g } CaSO4}{1 \text{ mole } CaSO4}$$

$$= 218 \text{ g } CaSO_4$$

A note on the definition of a Mole

The Mole is a standard SI unit for the amount of a substance. It is officially defines as 6.0221421×10^{23} formula units of a substance. (A formula unit is an atom of an elemental substance, a molecule of a molecular substance, or a formula unit of a more complex substance.)

The Mole has its origins with a hypothesis formulated by the Italian scientist Amedeo Avogadro (1776-1856). In 1811, Avogadro pointed out that:

"Gay-Lussac has shown in an interesting Memoir (Mémoires de la Société d'Arcueil, Tome II.) that gases always unite in a very simple proportion by volume, and that when the result of the union is a gas, its volume also is very simply related to those of its components. observed that gases combined in volume quantities in the same numerical ratio as the elements in a compound."

For example, two volumes of hydrogen gas would combine with one volume of oxygen gas to form water, H_2O.

Avogadro went on to state:

"But the quantitative proportions of substances in compounds seem only to depend on the relative number of molecules which combine, and on the number of composite molecules which result. It must then be admitted that very simple relations also exist between the volumes of gaseous substances and the numbers of simple or compound molecules which form them. The first hypothesis to present itself in this connection, and apparently even the only admissible one, is the supposition that the number of integral molecules in any gases is always the same for equal volumes, or always proportional to the volumes."

This second statement is the basis for Avogadro's Hypothesis (sometimes referred to Avogadro's Law) which can be stated, in modern terms as:

Equal volumes of different gases (at the same temperature and pressure) have the same numbers of particles.

In 1865, an Austrian scientist, Johann Josef Loschmidt (1821-1895), in a paper On the Size of the Air Molecules, calculated the diameter of an air molecule to be 0.000000969 mm. To do this, he had to calculate the number of molecules there were in a given volume of gas. That number was $2.687 \times 10^{19}/cm^3$ (equivalent, in modern terms, to 1.2×10^{24} molecules/mol).
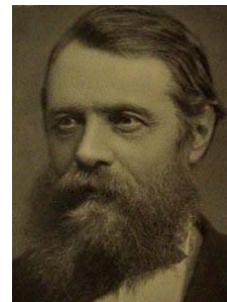
The term "Avogardo Number" or "Avogadro's Constant" was used by Jean Baptiste Perrin, (1870-1942), a French physicist, in a 1909 paper, Brownian Movement and Molecular Reality:

> "It has become customary to name as the gram-molecule of a substance, the mass of the substance which in the gaseous state occupies the same volume as 2 grams of hydrogen measured at the same temperature and pressure. Avogadro's proposition is then equivalent to the following:
>
> *"Any two gram-molecules contain the same number of molecules."*
>
> This invariable number N is a universal constant, which may appropriately be designated *Avogadro's Constant*."
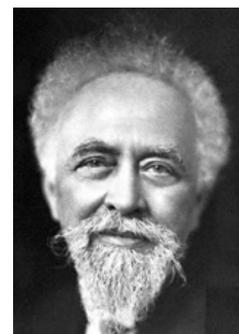
Perrin came up with a value of Avogadro's constant as 70.5×10^{22}.

Another calculation of Avogadro's number was made by American physicist Robert Millikan when he determined the charge on an electron. The charge on a mole of electrons had been known for some time and is the constant called the Faraday. Milliakn used the value of the Faraday as 9,650 electrostatic units and divided it by the electron charge of 4.774×10^{-10} electrostatic units to get a value of 6.062×10^{23}

Today, the best estimate of the value of a Faraday, according to the National Institute of Standards and Technology (NIST), is 96,485.3383 coulombs per mole of electrons. The best estimate of the charge on an electron based on modern experiments is $1.60217653 \times 10^{-19}$ coulombs per electron. If you divide the charge on a mole of electrons by the charge on a single electron you obtain a value of Avogadro's number of $6.02214154 \times 10^{23}$ particles per mole.

Avogadro's number is used in calculations when the number or mass of individual atoms or molecules is need.

Johann Josef Loschmidt

Jean Baptiste Perrin

Robert Millikan