Ch. 2. The periodic table: atoms and Elements

MATTER is everywhere around you, from the water you drink to the air you inhale. The matter is made of elements and elements are made of atoms. Even the atoms of an element can be different, having a distinct number of protons and neutrons. This chapter covers the principles of atomic structure. You will learn what makes an atom and will be able to quantify the particles that make atoms. Perhaps more importantly, you will also learn about the periodic table of elements and the different types of chemical formulas.

2.1 The periodic table

The periodic table (see Figure 2.1) is a chart containing all known elements arranged in increasing number of electrons per atom in a way that elements with similar chemical and physical properties are located together. The periodic table contains all existing elements–some of them are synthetic others are natural–that form the matter arranged in columns and rows. Every element has a different name accompanied by a symbol that represents its name. The tabular arrangement of elements in the form of rows and columns allows further classification of the elements according to their properties. This section will cover the different features of the periodic table.

Elements and Symbols Elements cannot be broken down into simpler substances. For example, aluminum is an element only made of aluminum atoms and if you analyze the composition of a piece of this metal you would only find aluminum atoms. Chemical symbols are one- or two-letter abbreviations that represent the names of the elements. Only the first letter is capitalized and if a second letter exists in the element's name, the second letter should be lowercase. For example, the chemical symbol for aluminum is Al, written as capital A and lowercase l.

Sample Problem 1

Give the symbol or name the following elements: C, Oxygen, N, Phosphorus, Au, Iron, Na and Iodine.

SOLUTION

The name of the element with symbol C is carbon, whereas the chemical symbol of oxygen is O. Similarly, N stands for nitrogen, whereas the chemical symbol of Phosphorus is P. The chemical symbol of Au is Gold. The chemical symbol of Iron is Fe and the chemical symbol of Iodine is I.

STUDY CHECK

Give the symbol or name the following elements: Ni.

▶Answer: Nickel

`Periods and groups` The periodic table (see Figure 2.1) contains all elements arranged in rows and columns. The horizontal rows are called *periods* and the vertical columns are called *groups or families*. For example, the first period contains hydrogen (H) and helium (He), whereas the second group contains Beryllium (Be), Magnesium (Mg), Calcium (Ca), Strontium (Sr), Barium (Ba) and Radium (Ra). There are seven periods (periods 1-7) and 18 groups. Some of the groups are labeled with an A (e.g. group 8A) whereas others are labeled with a B (e.g. group 8B). Group numbers can be found written with roman numbers and a letter (A or B) or with a more modern group numbering of 1-18 going across the periodic table. For example, group 2 (Mg-Ra) can also be called IIA, and group 13 (B-Ti) is also known as IIIA.

`Properties in the periodic table` The physical and chemical properties of some elements of the table (see Figure 2.1) are similar, and these similarities led to the organization of the periodic table. Elements in the same group share properties and for example, oxygen and sulfur have similar properties: both are reactive elements. Differently, the properties across periods change going from metals to nonmetals. For example, the properties of Li and Ne are very different, and lithium is a reactive metal whereas neon is a nonreactive gas.

`Metals, Nonmetals, and Metalloids` Overall, the elements of the periodic table (see Figure 2.1) can be classified as metals, nonmetals, and metalloids. Metals are those elements on the left of the table and nonmetals are the elements on the right of the table. The elements between metals and nonmetals are called metalloids and include only B, Si, Ge, As, Sb, Te, Po, and At. Metals are shiny solids and usually melt at higher temperatures. Some examples of metals are Gold (Au) or Iron (Fe). Nonmetals are often poor conductors of heat and electricity with low melting points. They also tend to be matt (non-shinny), malleable, or ductile. Some examples of nonmetals are Carbon (C) or Nitrogen (N). Metalloids are elements that share some properties with metals and others with nonmetals. For example, they are better conductors of heat and electricity than nonmetals, but not as good conductors as metals. Metalloids are semiconductors because they can act as both conductors and insulators under certain conditions. An example of metalloids is Silicon (Si) which should not be confused with silicone, a chemical employed in prosthetics.

Sample Problem 2

Answer the following questions: (a) Give the group and period of the following elements, and give the name: Ca, Ir, and C. (b) Classify as alkali metal, alkali earth metal, transition metal, halogen or noble gas, and give the name: Mg, Li, Co, He, F. (c) Classify as metal, nonmetal or metalloid, and give the name: Ba, N, Si.

SOLUTION

(a)The period and group of Ca (Calcium) is 2 (2A) and 4, respectively. The period and group of Ir (Iridium) is 9 (8B) and 6, respectively. The period and group of C (Carbon) is 14 (IVA) and 2, respectively. (b) Mg (Magnesium) is

> an alkali earth metal, whereas Li (Lithium) is a alkali metal. Co (Cobalt) is a transition metal. He (Helium) is a noble gas. F (Fluorine) is an halogen. (c) Ba (Barium) is a metal. N (Nitrogen) is a nonmetal. Si (Sillicon) is a metalloid.
>
> **STUDY CHECK**
>
> Answer the following questions: (a) Give the group and period of the following elements, and give the name: Cl. (b) Classify as alkali metal, alkali earth metal, transition metal, halogen or noble gas, and give the name: Ne. (c) Classify as metal, nonmetal or metalloid, and give the name: W.
>
> ▶Answer: (a) Chlorine: G 17 (VIIA) P3; (b) Neon Noble gas ; (c) Tungsten metal.

Classification of elements in terms of groups Some of the groups in the periodic table (see Figure 2.1) have specific names such as alkali metals, alkaline earth metals, transition metals, chalcogens, halogens, or noble gases. Alkali metals are the group 1A elements: lithium (Li), sodium (Na), potassium (K), rubidium (Rb), cesium (Cs), and francium (Fr). Alkali elements are soft and shiny metals, and they are also good conductors of heat and electricity, with low melting points. Alkali earth metals are group 2A (2) elements: beryllium (Be), magnesium (Mg), calcium (Ca), strontium (Sr), barium (Ba), and radium (Ra). Transition metals are the elements from groups 3 to 12 and they are located in the middle of the table. Chalcogens are group 6A (16) elements: oxygen (O), sulfur (S), selenium (Se), tellurium (Te), and polonium (Po). Halogens are group 7A (17) elements: fluorine (F), chlorine (Cl), bromine (Br), iodine (I), and astatine (At). Halogens are very reactive elements. Finally, noble gases are group 8A (18) elements: helium (He), neon (Ne), argon (Ar), krypton (Kr), xenon (Xe), and radon (Rn). They are inert and rarely combine with other elements in the periodic table, like a noble family: have you ever met a royal?

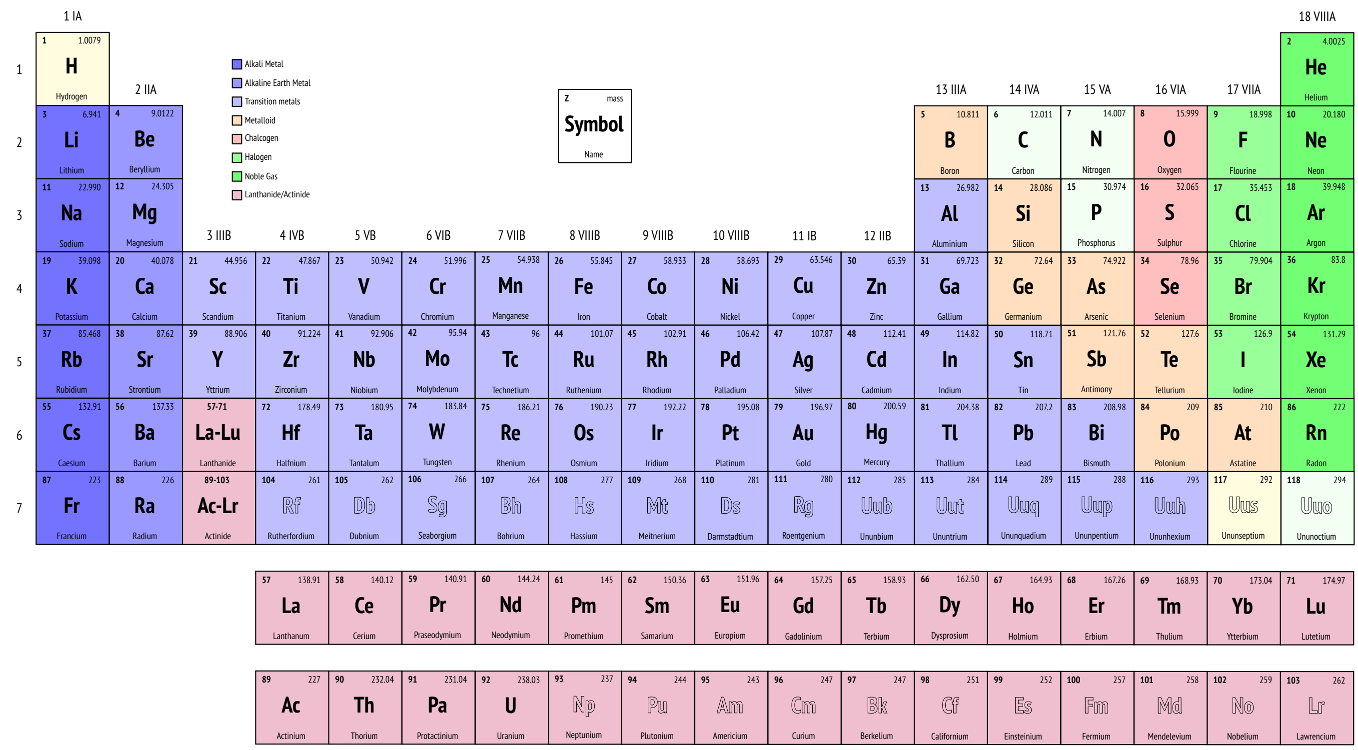


Figure 2.1 The periodic table of the elements

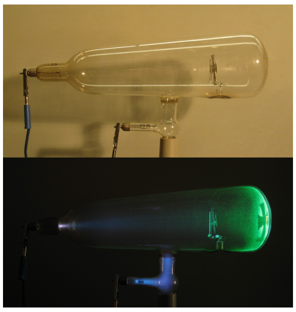
How to classify Hydrogen At first sight, hydrogen (H) may seem to be put in the wrong spot on the periodic table (see Figure 2.1). Although it is located at the top of

Group 1A (1), it is not an alkali metal, as it has very different properties. Thus hydrogen does not belong to the alkali metals, being nonmetal.

2.2 Early experiments of the atom

Scientists wondered about the nature of the atom and its structure for years. In a series of experiments carried out in the late nineteenth century, scientists such as J.J. Thomson, Henri Becquerel, and Ernest Rutherford gained insight into the nature and structure of the atom. These remarkable scientists and these creative experiments helped shape the view of the atom that we have nowadays.

▼A cathode tube



▼Millikan's apparatus

▼A plum pudding, with the electrons represented by the raisins

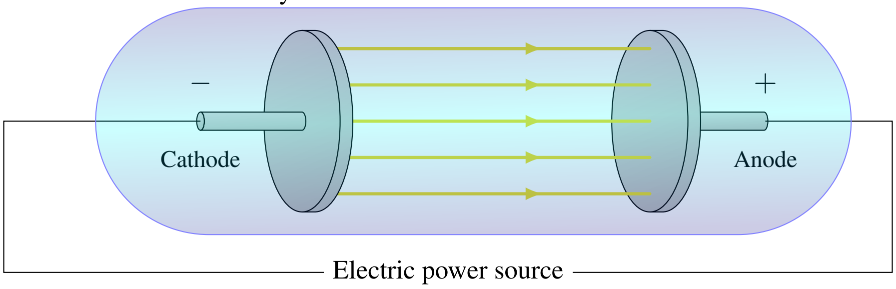


Figure 2.2 Cathode-ray tube made of two electrodes and a partially evacuated gas tube. The electrons, generated on the negatively charged electrode names cathode, excite the gas in the tube generating glow.

`Charge to mass ratio of an electron` The English researcher J.J. Thomson investigated electric discharges in partially evacuated tubes–tubes in which the air has been partially removed (See Figure 2.2); these tubes, made of a positive and negative electrode, are the base of old-fashion, bulky televisions. Thomson found that rays emanated from the negative electrode when applying high-voltage to these tubes. These rays were named cathodic rays as the negative electrode of the tube is called the cathode. Thomson also found that cathodic rays were repelled from the negative pole of an electric field. Hence, these rays were postulated to be a stream of negatively charged particles, now known as electrons. By studying the deflection of these rays by an electric field, Thomson was able to calculate the charge-to-mass ratio of an electron:

$$\boxed{\frac{e}{m_e} = -1.76 \times 10^8 C/g} \tag{2.1}$$

where:

e is the charge of an electron

m_e is the mass of an electron

Overall, the biggest of Thomson's discoveries was that all atoms are made of negatively charged particles. As atoms are charge-neutral, they are also made of positively charged particles. These observations led to a new atomic model, the *plum pudding model*, that envisioned atoms as a diffuse cloud of positive charges with negative electrons embedded in it. The name plum pudding comes from an English dessert that contains a raising spread. A different scientist, Robert Millikan, revealed the magnitude of the electric charge of the electron. Millikan used an apparatus that dispersed charged oil droplets falling under the influence of an electric field. Given the applied voltage and the droplet mass, Millikan was able to calculate the droplet charge. He found that the oil drop charge was always a whole number times the electron charge,

$$\boxed{e = 1.60 \times 10^{-19}\mathrm{C}} \tag{2.2}$$

where a Coulomb is a unit of charge. With the value of the charge-to-mass ratio of an electron and the electron charge, Millikan was also able to calculate the mass of an electron,

$$\boxed{m_e = 9.11 \times 10^{-31}\mathrm{kg.}} \tag{2.3}$$

`The atom nucleus` Ernest Rutherford carried out further experiments to validate the plum pudding model of the atom. He exposed a thin sheet of metal foil to α particles known to be massive and positively charged particles. According to the plum pudding model, the bulky α particles should have crashed through the thin foil and traversed through without being deflected. However, the results did not corroborate his expectations. Indeed, some particles traversed the film, whereas others were slightly deflected and some were strongly deflected at large angles. These observations did not corroborate the plum pudding model. However, they contributed to the creation of the modern atomic mode in which a large number of positive charges were concentrated at a point–called the nucleus– instead of being spread whereas the electrons move around the nucleus at large distances from it. The figure below represents the experiment carried out by Rutherford in which alpha particles were scattered on a think field made of gold.

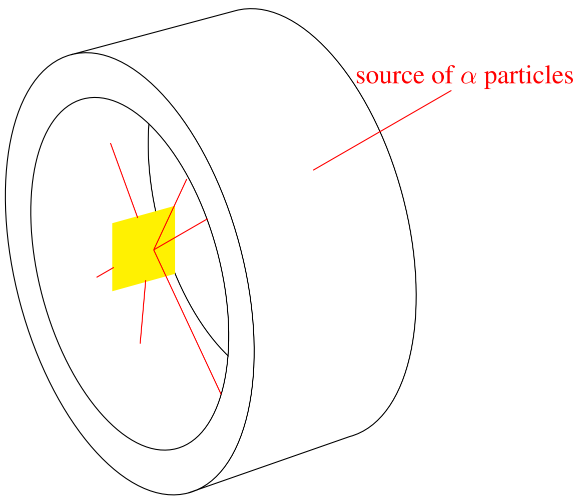


Figure 2.3 Rutherford's scattering: the elastic scattering of charged particles by the Coulomb interaction after a particle beam passed through a thin gold foil obstruction.

`Radiation` In the last part of the nineteenth century, scientists came to the discovery that some materials were able to produce high-energy radiation. Among the scientist working in this field, Henri Becquerel discovered that pitchblende, a mineral containing uranium, was able to produce an image on a photographic plate in the absence of light. In the early twentieth century, three different types of radiation were discovered: alpha radiation, beta radiation, and gamma radiation. Further studies revealed that gamma radiation was made of gamma particles, high-energy radiation, whereas beta radiation was made of high-energy electrons. Alpha particles were found to be positively charged, with a charge twice the charge of an electron and a mass 7300 times that of the electron. These particles were indeed Helium's nucleus, resulting from removing electrons from atoms of Helium.

2.3 The atom

Atoms are the smallest piece of an element that retains their characteristics. They are the building blocks of matter. This section covers the structure of the atom. You will learn how to calculate the number of subatomic particles that made an atom and how to differentiate atoms of an element–all atoms of an element are not equal.

`Atomic Structure` An atom is an electrically neutral, spherical entity made of a nucleus surrounded by negatively charged electrons. Atoms contain three atomic particles: the proton, neutron, and electron. Protons have a positive charge (+), whereas electrons carry a negative charge (–). Both electrons and protons have the same charge in magnitude but with opposite signs. Neutrons on the other hand are neutral, and they have no electrical charge. Protons and neutrons are located in the core of the atom, which is called the nucleus, and account for the mass of the atom. The only exception is the hydrogen atom, the smallest element, with just one proton in the nucleus. Electrons are delocalized in the exterior part of the atoms. They are not necessarily located in a specific spot and their existence spreads in the area next to the nucleus. Electrons move rapidly and are spread and held by nuclear attraction. Atoms are neutral without a charge as the number of electrons and protons are the same. Some atoms have a positive charge, resulting in removing electrons, and we call these cations. Others–called anions–can have a negative charge as a result of accepting a negatively charged electron. The mass of a proton or neutron is 2000 times larger than the mass of an electron and the atom's diameter is more than 10000 times the diameter of its nucleus. The nucleus is very dense being 99% of an atom's mass while occupying a small volume.

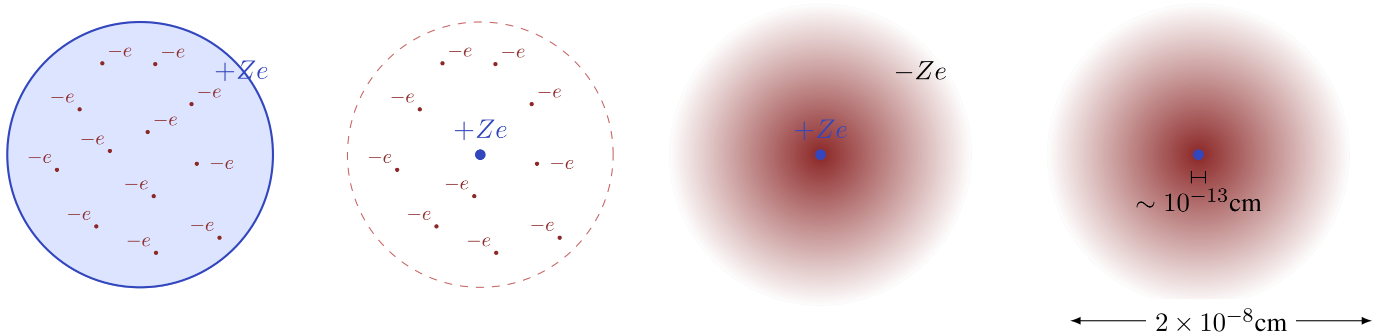
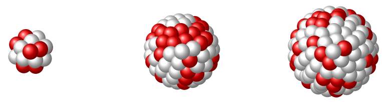


Figure 2.4 Three models of the atom. From left to right: the plum puding model, the updated plum pudding model according to Rutherford's observations, (two right images) the modern atomic model. Z is the atomic number of the atom.

Elements are made of atoms, and each atom of an element is characterized by an atomic number (Z) and a mass number (A). The atomic number (Z) of an element indicates the number of protons in an atom. This number can be easily located in the periodic table (see Figure 2.1). All atoms of an element have the same atomic number, whereas the atomic number of different elements differ. For example, Carbon has an atomic number of Z=6, whereas Oxygen has an atomic number of Z=8. The mass number (A) of an element indicates the combined number of protons and neutrons. Mass numbers can not be found in the periodic table. More importantly, different atoms of the same element can have different mass numbers. For example, a Carbon atom made of 6 neutrons and 6 protons has a mass number of A=12. Both A and Z for an atom X are indicated in the following form called isotope notation:

$$\text{Atomic and mass number } {}^{A}_{Z}X$$

As an example, the notation ${}^{24}_{12}Mg$ means that the atomic number of Mg is Z=12 and the mass number is A=24. Using the isotope notation, one can quickly identify the number of protons, neutrons, and electrons in an atom. As the atomic number is always indicated on the bottom part (e.g. Mg has 12 electrons). At the same time, the number of electrons and protons in a neutral atom is the same–neutral means an atom without a charge. The number of neutrons of an isotope can be computed by subtracting the atomic number from the mass number. Below you can find three different atoms, an atom of Carbon with 12 protons and neutrons, a larger atom of Calcium with 44 protons and neutrons, and an even larger atom of Gold with 197 protons and neutrons.



${}^{12}_{6}C$ ${}^{44}_{20}Ca$ ${}^{197}_{79}Au$

Sample Problem 3

Calculate the number of protons, neutrons and electrons of the following atoms:

(a) ${}^{27}_{12}Mg$ (b) ${}^{22}_{10}Ne$ (c) ${}^{20}_{10}Ne$

SOLUTION

(a) ${}^{27}_{12}Mg$ has 12 electrons (Z=12) and 12 protons as well (the number of electrons and protons are the same if the atom is neutral), and 15 neutrons, as 27-12=15. (b) ${}^{22}_{10}Ne$ has 10 electrons and 10 protons, and 12 neutrons. (c) ${}^{20}_{10}Ne$ has10 electrons and 10 protons, and 10 neutrons as well.

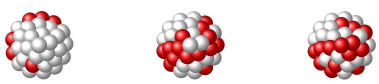
STUDY CHECK

Calculate the number of protons, neutrons and electrons of the following atoms:

(a) ${}^{32}_{16}S$ (b) ${}^{34}_{16}S$ (c) ${}^{36}_{16}S$

▶Answer: (a) 16p, 16e and 16n; (b) 16p, 16e and 18n; (a) 16p, 16e and 20n.

Isotopes All atoms of an element have the same atomic number but may differ in terms of mass number. Isotopes are atoms of the same element with different numbers of neutrons and therefore with different mass numbers but with the same atomic number. For example: ${}^{24}_{12}Mg$, ${}^{25}_{12}Mg$ and ${}^{26}_{12}Mg$ are three isotopes of Mg. ${}^{27}_{12}Mg$ is heavier than ${}^{24}_{12}Mg$ as it contains more neutrons and protons in the nucleus. Most elements occur in nature in a particular isotopic composition, and each of the isotopes has a specific proportional abundance. For example, the abundance of ${}^{24}_{12}Mg$ is 79%, and the abundance of ${}^{25}_{12}Mg$ and ${}^{26}_{12}Mg$ is 10% and 11%, respectively. This means, ${}^{24}_{12}Mg$ is more abundant than for example ${}^{26}_{12}Mg$.



${}^{24}_{12}Mg$ ${}^{25}_{12}Mg$ ${}^{26}_{12}Mg$

Another example of isotopes can be found in Carbon, with two naturally occurring isotopes. In the case of charged atoms, we have the cations have fewer electrons than their corresponding atom, whereas anions have more electrons, both based on their charge. The mass of an atom is measured relative to the mass of an atomic standard, the Carbon-12 atom, whose mass is defined as 12 atomic units of mass, amu. For example, the mass of ^{1}H is 1.008 amus. The term atomic unit of mass has been renamed to dalton (Da). Therefore, the mass of ^{1}H is 1.008 amus or 1.008 Da. The atomic mass is a relative unit of mass equivalent to 1.66054×10^{24}g.

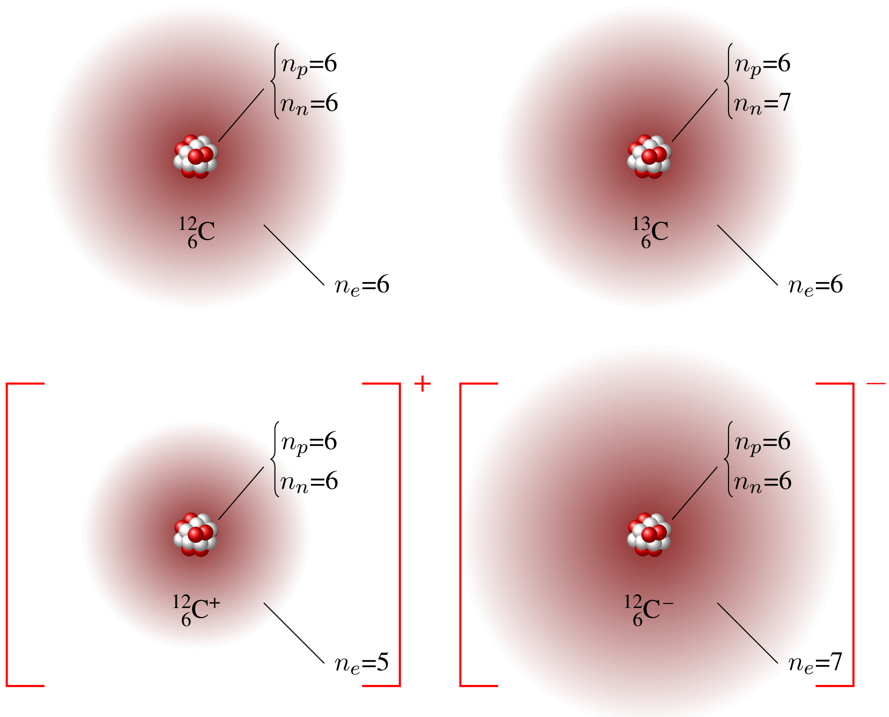


Figure 2.5 Representations of four different atoms, two neutral atoms on top and two ions on the bottom.

`Average atomic mass` As atoms are made of numerous isotopes–this means different atoms of the same element but with a different number of neutrons and hence different weights. The average atomic mass (also called atomic weight) represents the mass of the atoms of an element and results from all existing isotopes taking into account their abundance. It is the average of the masses of the naturally occurring isotope weighted according to their abundance expressed in atomic mass units or daltons. We can think of % *relative abundance*, and for example, the % relative abundance of ^{1}H is 99%. But we can also think of *fractional abundance*, that in the case of ^{1}H would be 0.99. For an element with n isotopes each with different masses (A_1, A_2, ..., A_n) and different fractional abundances (f_1, f_2, .., f_n), the atomic mass is given by

$$\text{Atomic mass} = \sum_{i=1}^{n} A_i \cdot f_i = A_1 \cdot f_1 + A_2 \cdot f_2 + \cdots + A_n \cdot f_n$$

Note that when adding the fractional abundances of all isotopes, one should obtain a value of one:

$$\sum_{i=1}^{n} f_i = f_1 + f_2 + \cdots + f_n = 1$$

Atomic masses can be simply found in any periodic table (see Figure 2.1) for each element. For example, the atomic mass of oxygen (O) is 15.999 amu and the atomic mass of nitrogen (N) is 14.007 amu. The atomic mass found in the periodic table is an average that results from including the mass of the different isotopes and their abundance. Table 2.1 lists the relative abundance of a series of common isotopes.

Sample Problem 4

Naturally occurring copper (Cu) consists of 69.17% ^{63}Cu and 30.83% ^{65}Cu. The mass of ^{63}Cu is 62.939598 amu, and the mass of ^{65}Cu is 64.927793 amu. What is the atomic mass of copper?

SOLUTION

The weighted average is the sum of the mass of each isotope times its fractional abundance. We have that the isotope ^{63}Cu has a mass of 62.939598 amu and an abundance of 69.17%, that is the same as 0.6917. At the same time, the isotope ^{65}Cu has a mass of 64.927793 amu and an abundance of 0.3083. After adding both contributions, we have:

$$62.939598\,amu \times \frac{69.17}{100} + 64.927793\,amu \times \frac{30.83}{100} = 63.55\,amu$$

We can use the table below to obtain the final result:

Isotope	m_i (amu)	f_i	$m_i \times f_i$
^{63}Cu	62.939598	0.6917	43.53
^{65}Cu	64.927793	0.3083	20.02
Average atomic mass (amu)			$= \sum m_i \times f_i$ =63.55

STUDY CHECK

Lithium is made up of two isotopes, Li-7 (7.016003 amu) and Li-6 (6.015121 amu). Calculate the percent abundance of each isotope knowing that lithium's atomic weight is 6.94 amu.

▶Answer: 7.59% and 92.41%.

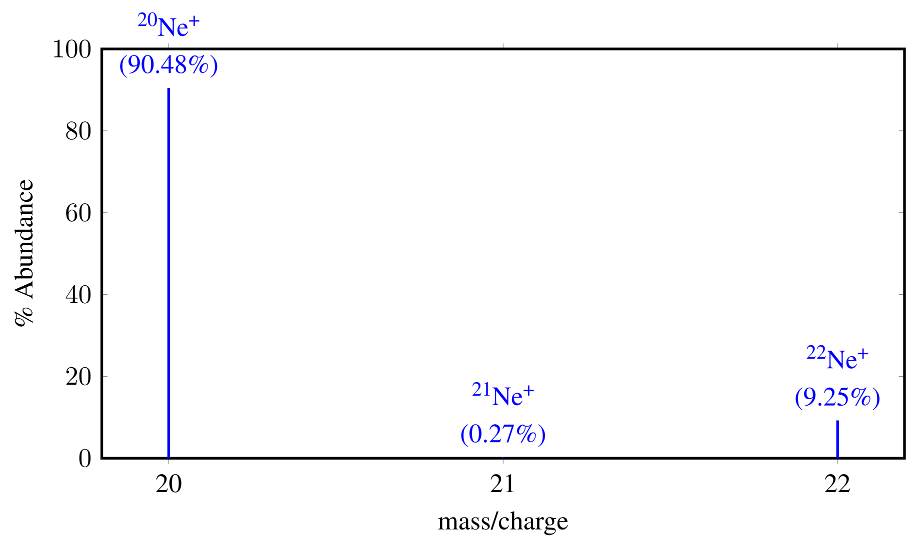


Figure 2.6 Mass spectra of Neon with three peaks corresponding to three different isotopes with different relative abundance.

`Mass spectrometry` Mass spectroscopy is a technique used to determine the isotopic composition of an element. With this technique, we can measure the relative mass and abundance of small atomic particles. In this technique, high-energy electrons collide with atoms or molecules to form ionized atoms. For example, if Ne would be analyzed, high energy electrons would produce Ne^+ characterized by its mass charge ratio, m/e. Different isotopes would have different m/e ratios. The positively charged particles produced after the impact would be attracted toward a series of negatively charged plates with slits in them. Some of these particles would pass through the slits into an evacuated tube exposed to the effect of a magnetic field. As the particles enter the evacuated region their paths are bent so that the lightest particles (low m/e) are more deflected than the heaviest particles (high m/e). Finally, the particles would stick to a detector recording their relative position and abundance. The spectrometer also provided the mass ratio of an isotope with respect to the mass standard, ^{12}C.

Table 2.1 Isotope abundance of some elements

Element	Isotope	% Abundance	Element	Isotope	% Abundance
Hydrogen	^{1}H	99.9885%	Silicon	^{28}Si	92.2297%
	^{2}H	0.0115%		^{29}Si	4.6832%
Helium	^{3}He	0.000137%		^{30}Si	3.0872%
	^{4}He	99.999863%	Sulfur	^{32}S	94.93%
Lithium	^{6}Li	7.59%		^{33}S	0.76%
	^{7}Li	92.41%		^{34}S	4.29%
Boron	^{10}B	19.9%		^{36}S	0.02%
	^{11}B	80.1%	Chlorine	^{35}Cl	75.78%
Carbon	^{12}C	98.93%		^{37}Cl	24.22%
	^{13}C	1.07%	Argon	^{36}Ar	0.3365%
Nitrogen	^{14}N	99.632%		^{38}Ar	0.0632%
	^{15}N	0.368%		^{40}Ar	99.6003%
Oxygen	^{16}N	99.757%	Potassium	^{39}K	93.2581%
	^{17}O	0.038%		^{40}K	0.0117%
	^{16}O	0.205%		^{41}K	6.7302%

2.4 An introduction to molecules

The periodic table (see Figure 2.1) contains all elements in nature. At the same time, elements combine to form molecules. For example, in the air there are traces of Argon–this is an element–and also water, a molecule (H_2O) that results from the combination of two elements, hydrogen (H) and oxygen (O). This section will first introduce some of the properties of molecules, without paying attention to their chemical names that will be covered in the following chapters.

Molecular weight Here are two examples of molecules: molecular oxygen O_2 and molecular nitrogen N_2. How do we interpret these formulas? The subscript "2" indicates that each molecule contains two atoms. For example, a O_2 molecule is made of two oxygen atoms O. At the same time, the weight of a set of molecules is called the molecular weight (MW). However, you will find different terms to refer to the same property such as molecular mass, molar mass, or formula unit mass. All these terms indeed mean the weight of a large set of molecules. We can calculate the MW by adding the weight of each atom that forms the molecule taking into account the number of atoms of each element present in the molecule. The units of molecular weight are the same as the units of atomic weight: amu, atomic mass units.

Sample Problem 5

Calculate: (a) The atomic weight of O; (b) the molecular mass of molecular oxygen, O_2

SOLUTION

(a) According to the periodic table the atomic weight (AW) of O is 15.999 amu.
(b) The molar mass of O_2 is the result of adding the atomic masses of 2O atoms, that is 31.998 amu, close to 32 amu.

STUDY CHECK

Calculate the molar mass of water H_2O and ammonia, NH_3

▶Answer: 18 and 17 amu.

Mass percent composition of a compound Look at these two molecules: C_2H_2 and C_2H_6. They contain different amounts of hydrogen. We quantify the amount of an element in a compound using the mass % composition. The mass % of an element in a compound is the mass of the element concerning the molecular weight of the molecule in percent form. Mind that you have to take into account the molecular indexes in the compound as C_2H_2 is made of 2H and C_2H_6 is made of 6H. For example, given that the molar mass of C_2H_2 is 26 amu, the mass % of hydrogen in C_2H_2 would be:

$$\%_H \text{ in } \mathrm{C_2H_2} = \frac{2 \cdot AW(H)}{MW(\mathrm{C_2H_2})} \times 100 = \frac{2 \cdot 1}{26} \times 100 = 7.7\%$$

Similarly, the mass % of C would be:

$$\%_C \text{ in } \mathrm{C_2H_2} = \frac{2 \cdot AW(C)}{MW(\mathrm{C_2H_2})} \times 100 = \frac{2 \cdot 12}{26} \times 100 = 92.3\%$$

By adding the mass % of all elements in a molecule we should obtain 100.

$$\%_H \text{ in } \mathrm{C_2H_2} + \%_C \text{ in } \mathrm{C_2H_2} = 100$$

Sample Problem 6

Calculate the mass % composition for each element of glucose, $C_6H_{12}O_6$.

SOLUTION

We first need the molecular weight of glucose, $C_6H_{12}O_6$, that is: $6 \cdot 12 + 12 \cdot 1 + 6 \cdot 16 = 180$ amu. Now we can calculate the mass percent of carbon, hydrogen and oxygen:

$$\%_C \text{ in } \mathrm{C_6H_{12}O_6} = \frac{6 \cdot 12}{180} \times 100 = 40\%$$

$$\%_H \text{ in } \mathrm{C_6H_{12}O_6} = \frac{12 \cdot 1}{180} \times 100 = 6.6\%$$

By subtraction, we have that $\%_C$ in $C_6H_{12}O_6 = 53.4$.

STUDY CHECK

Ureas $CO(NH_2)_2$ is a colorless crystalline compound excreted in urine, product of protein metabolism in mammals. Calculate the mass % composition for each element of urea.

▶Answer: $20\%_C$, $26.7\%_O$, $46.7\%_N$, $6.6\%_H$.

2.5 Empirical and molecular formula of a chemical

There are two different types of formulas: molecular formulas and empirical formulas. Empirical formulas (EFs) are simplified formulas resulting from an experiment, whereas molecular formulas (MFs) are exact formulas of molecules. For example, the molecular formula of hydrogen peroxide, a mild antiseptic used on the skin to prevent infection of minor cuts, is H_2O_2 as the hydrogen peroxide molecule is made of two oxygen and two hydrogen atoms. Differently, the empirical formula of the same chemical is HO, being this the result of the simplification of H_2O_2. One can obtain empirical formulas simply by dividing the molecular formula by the smallest integer number, of course, given you know the molecular formula. The word empirical means "from an experiment", and the use of empirical formulas comes from the fact that the formulas of all chemicals come from experiments, and from experiments, one normally can only obtain ratios of atomic composition.

Sample Problem 7

From the following formulas identify the empirical and molecular formulas: P_4O_{10}, C_3H_6O, N_2O_4 and C_5H_{11}.

SOLUTION

Empirical formulas are simplified versions of molecular formulas. For example, C_3H_6O and C_5H_{11} are empirical formulas. Differently, P_4O_{10} and and N_2O_4 are molecular formulas.

STUDY CHECK

Given the following molecular formulas, obtain the corresponding empirical formula: P_4O_{10}, N_2O_4 and $C_6H_{18}O_3$.

▶Answer: P_2O_5, NO_2 and C_2H_6O.

Molecular weight of empirical formulas and molecular formulas

The molecular weight of an empirical formula and its corresponding molecular formula are related by the following formula:

$$\boxed{n = \frac{MW_{MF}}{MW_{EF}}}$$

where:

MW_{EF} is the molecular weight of the empirical formula

MW_{MF} is the molecular weight of the molecular formula

n is an integer number such as 1, 2, 3...

Understanding the formula above is simple. On one hand, the MW of a molecular formula H_2O_2 is 34 amu. On the other hand, the molecular weight of the empirical formula of the same chemical HO is 17 amu. If we do $34/17$ we would obtain 2, as we need to multiply HO by two to obtain H_2O_2. As a final note, mind that empirical formulas are just simplified formulas. So when we think about the molecular weight of a chemical we normally have a molecular formula in mind. Let us work on an example.

Sample Problem 8

Given that the empirical formula of dichloroethane is $ClCH_2$ and the molecular weigh of the chemical is 98amu, calculate the molecular formula of dichloroethane.

SOLUTION

Given the empirical formula of dichloroethane one can think of many different molecular formulas, for example: $Cl_3C_3H_6$ or $Cl_2C_2H_4$. From these, and many other, there is only on real molecular formula. How do we calculate the real molecular formula? By comparing the MW of the molecular and empirical formula we can figure out the number of time we need to multiply the MF to obtain the EF. We know the MW is 98amu. Using the EF we can also calculate a MW: $35 + 12 + 2 \cdot 1 = 49$ amu. If we compare both number using the formula:

$$n = \frac{MW_{MF}}{MW_{EF}}$$

we have: $n = 98/49$ and solving we have $n = 2$. Therefore the MF is: $Cl_2C_2H_4$.

STUDY CHECK

The empirical formula of dinitrogen tetroxide, a red-brown liquid with an unpleasant chemical odor, is NO_2 and the molecular weigh of the chemical is 92 amu. Calculate the molecular formula of dinitrogen tetroxide.

▸Answer: N_2O_4.

2.6 Determining empirical formulas

We said that the formula of a chemical that takes into account the correct number of atoms in a molecule is the molecular formula and therefore the real molecular weight of a chemical comes from these formulas. Empirical formulas are obtained from experiments in which a chemical is fragmented and analyzed so that the elements in the molecule and the mass percentage of each element are determined. Molecular formulas are obtained by using the molecular weight of the chemical and the empirical formula. Mind that the formula of a chemical that takes into account the correct number of atoms in a molecule is the molecular formula and therefore the real molecular weight of a chemical comes from these formulas. Let us work on an example to learn the procedure of obtaining molecular formulas.

Calculating molecular formulas We want to calculate the empirical formula of a chemical given that the chemical contains 2.8 g of nitrogen and 6.4 g of oxygen. To calculate the EF we will set up a table like the one presented below.

Empirical Formula Calculation		
	N	O
Grams	2.8g	6.4g
AW	14	16
Grams/AW	0.2	0.4
÷ by smallest	1	2
Formula	N_1O_2=NO_2	

In each column, we will add each of the elements that form the molecule. In the first row, we will include the grams of each element (sometimes this information is given in terms of mass %), in the second we will divide the grams of each element by its atomic weight (AW(N)=14amu,AW(O)=16amu). Among all numbers of the second row (in this example 0.2 and 0.4), we will select the smallest number (0.2). Once we have the smallest, we will divide all numbers by the smallest, and that will give us round numbers (1 and 2); these will be the numbers in an empirical formula: NO_2.

Sample Problem 9

The mass percentage composition of a compound is: 18.59% O, 37.25% S, and 44.16% F. Calculate its empirical formula.

SOLUTION

We will set up the the molecular formula table, knowing that the percentage are mass percentages, that is the mass of each element in the chemical, hence they should go in the grams row. Also the atomic weights of O, S and F are 16, 32 and 19 amu.

Empirical Formula Calculation			
	O	S	F
Grams	0.1859g	0.3725g	0.4416g
AW	16	32	19
Grams/AW	0.0116	0.0116	0.0232
÷ by smallest	1	1	2
Formula	OSF_2		

STUDY CHECK

What is the empirical formula of a compound if a sample contains 10.28 g of C, 1.71 H and 12.71 g of oxygen?

Answer: CH_2O.