

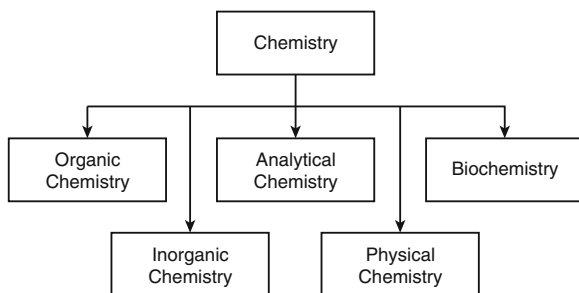
## Chapter 2

# Chemical Organic Compounds

For centuries, human beings have found inspiration in nature, from macro-scale to micro-scale. Animals have been inspiring designs of cars, robotics, and even computational algorithms based on their behaviors. Some new super tough materials got inspired in deer antlers. Environmental analysis of pressure, temperature or humidity have been inspiring new ways of greenhouses. Shapes of nature have been inspiring on painting, digital art, or sculpture. Chemical products like waterproofing sprays were inspired on specific nanostructures of lotus leaves. Also, burdock seeds inspired the well-known hook-and-loop fastener.

In particular, scientists and researchers take advantage of natural inspiration because nature has shown that it can adapt itself to better response of changes and can reach feasible solutions to problems like better configurations of structure of matter, or animal survival in ecosystems. In fact, nature tends to optimality in all different ways. For instance, consider atom-structures that tend to minimize energy in bonds, but also preserve particular characteristics depending on atom relationships. To this end, the notion of the latter will be highly important through this book because the study of chemical organic compounds inspires artificial organic networks.

For instance, consider a given physical system with some input and output signals. Then, the supervised artificial organic networks technique can model the system using signal information to build a structure made of atoms that are clustered in molecules. In fact, these molecules will be used to enclose related information found in the signals of the system. Moreover, if molecules cannot approximate completely the behavior of the system, they can be joined together forming complex molecules (referred also as compounds). At last, compounds can also mix them up forming mixtures of molecules that represent linear combinations of behaviors of subsystems, giving an organized structure approximating the overall system. Actually, this structure will be referred as an artificial organic network because it is inspired on carbon based networks, especially studied on organic chemistry, that present highly stable molecules due to the electronegativity of carbon atoms. Interesting, an artificial organic network presents characteristics like structural organization, clustering



**Fig. 2.1** Branches of chemistry

information, inheritance of behavior, encapsulation of data, and stability in structure and response.

Thus, this chapter introduces fundamentals on organic chemistry to deeply understand artificial organic networks. In particular, basic concepts of organic compounds are described from the point of view of structural stability and energy minimization. In addition, classification of organic compounds is outlined. Finally, hydrocarbons, the most stable organic compounds in nature, are described.

## 2.1 The Importance of Organic Chemistry

Chemistry studies the matter, its properties and the laws that govern it. As known, chemistry is divided into five branches: organic chemistry, inorganic chemistry, analytical chemistry, physical chemistry, and biochemistry, as shown in Fig. 2.1. For instance, organic chemistry is the study of the compounds of carbon while inorganic chemistry is the study of all other compounds [10]. Analytical chemistry is the study of methods that determine and identify elements in compounds. Physical chemistry applies physics to chemistry and it is the study of thermodynamics and kinetics of chemical reactions, and biochemistry is the study of chemical processes inside living organisms.

Centering on organic chemistry, it is very important in different ways. Looking around, organic products are present daily like cleaning accessories as soaps, shampoos or perfumes; they are also present in food as proteins, lipids and carbohydrates that give and store energy, that are included in structural formation, that transport other molecules, or that regulate growth in living organisms. In fact, all compounds responsible of life are organic substances denominated biomolecules, e.g. proteins, lipids, carbohydrates; but also nucleic acids, complex molecules involved in genetics, are considered part of them [1, 3, 4].

It is interesting how compounds made of carbon atoms can define millions and millions of different organic compounds. Actually, carbon atoms can interact among them to form chains and rings, giving the opportunity of changing chemical properties

of compounds [4]. This is possible because their bonds with other atoms are very strong in comparison with other atomic interactions, as explained later in this chapter.

Moreover, organic chemistry is not only present in living organisms, it is also involved in human health technologies like the development of new drugs or the study of materials, e.g. hypoallergenic materials, used in prothesis or cookware coating; production of food; development of cancer treatments as the so-called “sharp-shooter” drugs. Also, it is widely used for developing new materials applied in space. Other industrial applications of organic compounds are: solvents like degreasers or dry cleaning products, chemical gums for wood like latex or white glue, plastics like toys or plastic coatings, etc.

Then, organic chemistry is generating new tendencies in technology and applied sciences. For example, consider the development of alternative energy sources as biofuels that can be produced from plants or organic waste; or consider organic photo-sensors that convert light in electrical signals to capture images in cameras. Furthermore, in computer sciences, organic chemistry is inspiring DNA-computing to solve hard problems with strands of DNA, or the organic computing paradigm that inherits organic properties to multiagent systems.

In addition, current trends of organic chemistry are related to green chemistry that encourages the usage minimization of hazardous substances to the environment; applications of fullerenes (molecules completely made of carbon atoms) in strength of materials, biology, treatments for industrial wastewater in the field of nanotechnology, architecture inspiration, conductivity materials, antiviral production, etc.; other trends like solid state materials, organic nanostructures, liquid crystals, organic dyes, organometallic applications to polymeric production, agrochemistry, and so forth.

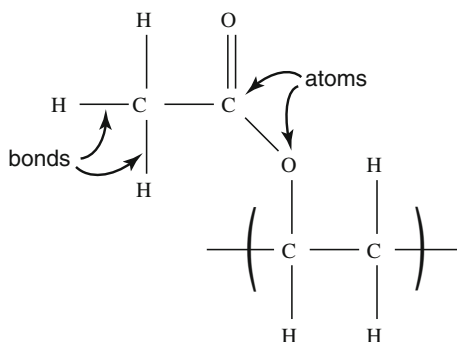
On the other hand, it is well known that organic chemistry influences the global economy with hydrocarbons, specially in the production of petroleum, and the industry of polymers [3]. Thus, organic chemistry is highly important in the daily life, from the study of living organisms to medical applications, through the economical and technological impact.

## 2.2 Basic Concepts of Organic Compounds

Organic chemistry is the study of the compounds of carbon [3, 10]. Interestingly, most of these compounds consist of carbon and a few of other elements like hydrogen, oxygen, nitrogen, phosphorus, sulfur, and halogens (fluorine, chlorine, bromine, iodine, astatine). In fact, organic compounds have important physical and chemical properties derived from carbon bonding to itself and the specialization of the few other elements, like the strength of structures or the effecting of heat.

In the following sections, physical properties are associated to the structure of organic compounds while chemical properties to the behavior of them. Notice that this review is organized in order to highlight the role of energy stabilization in organic compounds.

**Fig. 2.2** Example of the molecular structure of polyvinyl acetate, an organic compound used in white glue



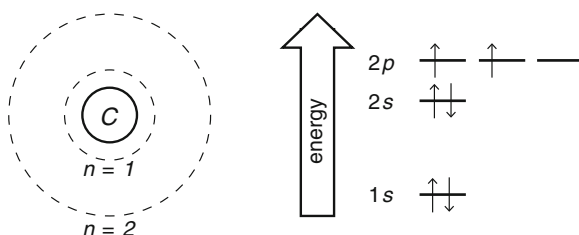
### 2.2.1 Structural Definitions

Organic compounds are constituted with basic units called atoms. When atoms interact among them, they form molecules and compounds, as shown in Fig. 2.2. Thus, the structure of organic compounds considers the set of atoms and the ways they are bonded. But also, energy minimization and geometric configuration play an important role in the structure [5]. Following, basic components and interactions of chemical organic compounds are summarized.

#### 2.2.1.1 Atoms

The basic unit of organic compounds is the atom [4, 5]. Each atom is a set of charged particles including protons, electrons and the neutral particles so-called neutrons. Roughly, any atom has protons and neutrons joined together at its nucleus and the latter is surrounded by a set of electrons. The sum of protons and neutrons is equals to the mass number of an atom. In addition, the number of protons in the nucleus is referred as the atomic number. Hence, different atoms have different atomic numbers. The well-known periodic table summarizes this and other concepts about atoms. Thus, different atoms have distinct physical characteristics. In the sense of this book, the distinction of an atom is limited to the atomic number, and different atoms refer to different behaviors due to their physical characteristics.

For instance, the model of atoms assures that they have a particular way to distribute their electrons known as electron configuration [3, 4]. It assumes that electrons can only orbit in specific spaces called energy shells. Additionally, shells are divided into subshells (i.e. *s*, *p*, *d* and *f*) in which electrons are grouped in orbitals. Finally, each orbital can be occupied by at most two electrons. However, electrons might represent an infinite set of configurations. In that sense, studies in chemistry and quantum mechanics reveal that there is an electron configuration in which electrons preserve the minimum energy of the atomic system, so-called the ground-state (see Sect. 2.2.2.3).



**Fig. 2.3** Simple model of the carbon atom and its energy-level diagram

Atoms are also characterized by valence electrons. These kinds of electrons are the ones which conform to the last energy shell defined in the atom. Particularly, this energy shell is called outer shell. Since electrons need some energy to be in shells, the ground-state assures that energy minimization occurs when electrons follow the quantum chemistry principles (see Sect. 2.2.2.3). Otherwise, atoms are in an excited state.

Basically, noble gases (e.g. helium, neon, argon, krypton, xenon, radon) are the only atoms with minimum energy per shell. Then, atoms must satisfy a chemical rule that states atoms in ground-state which do not have an entire outer shell (there are some valence electrons but not all of them) need more electrons in order to complete it. This is the basis of atomic interactions in organic chemistry: ionic interactions and covalent bonds, treated later in this chapter. Figure 2.3 shows a simple model and the energy-level diagram of carbon atom.

### 2.2.1.2 Molecules

A set of two or more atoms acting as a single unit is called a molecule. As mentioned previously, atoms need to complete the outer shell with electrons; thus, creation of molecules is one mechanism to do that. Three important types of molecules are defined following:

**Elements.** These molecules are made of like atoms, e.g. hydrogen element, because atoms are not found isolated in nature. Elements can be classified into three categories:

- Metals.* Physically, they are solid at room temperature (except mercury), they can also be shiny, malleable and ductile, and they serve as conductors of electricity. Chemically, they react losing electrons.
- Nonmetals.* Physically, they are the opposite of metals. Chemically, they react gaining electrons. These elements are the only ones present in chemical organic compounds.
- Metalloids.* They have a hybrid behavior combining metal and non-metal properties.

**Compounds.** They are molecules made of other molecules when reacting two or more of them. In the general case, a compound is made up elements proportionally to its mass. For instance, organic compounds are made of carbon atoms. If there are no carbon atoms, then compounds are considered as inorganic.

**Functional groups.** These molecules are made of a carbon atom bonded with one of the other atoms allowed in organic compounds. Functional groups are important because organic compounds are classified based on them; chemical reactions act on them in order to form other stable compounds, simple or complex; and, they are basis for naming organic compounds.

### 2.2.1.3 Chemical Bonding

In molecules, chemical bonding refers to the relationship among atoms. In fact, this process is based on charged particle attraction. In chemistry, two main chemical bondings are present: ionic interactions and covalent bonds.

**Ionic interactions.** A metal element tends to lose electrons while a nonmetal element tends to gain electrons. Thus, ionic interaction is present into a metal-and-nonmetal reaction. Particularly to organic compounds, these chemical bondings are not present.

**Covalent bonds.** When two nonmetal atoms are interacting, they cannot lose or gain electrons. Thus, they share electrons of their outer shells. Due to the set of atoms in organic compounds, covalent bonds will be considered through this book.

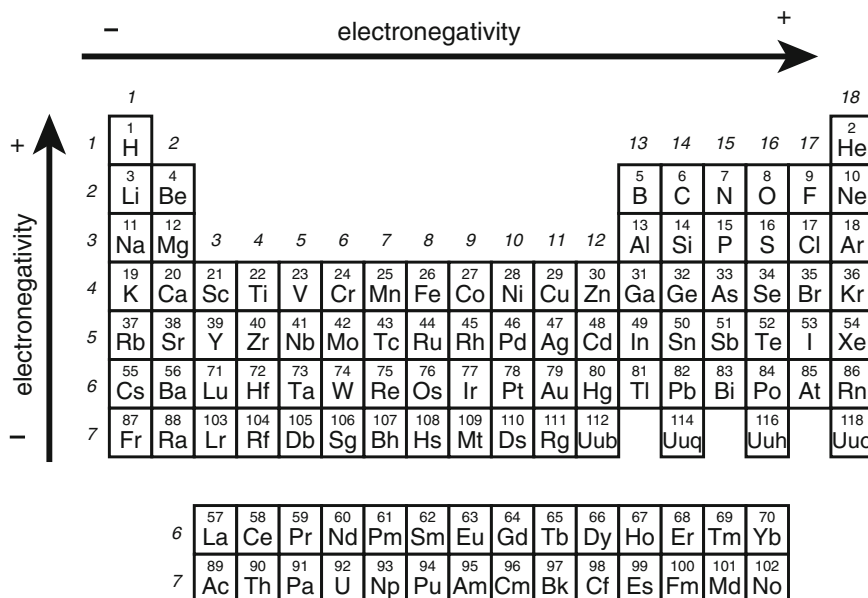
In both cases, chemical bonding is explained by electronegativity which it is presented in Sect. 2.3.

## 2.2.2 Chemical Definitions

The study of interactions of atoms and molecules are based on chemical rules and properties. Depending on them, organic compounds have specific characteristics and behaviors. In the following section, chemical principles are depicted in order to understand the behavior of molecules and chemical bonding [5].

### 2.2.2.1 Electronegativity

In chemistry, the notion of tendency of atoms to attract electrons is a chemical property associated to atoms named electronegativity [4, 5]. For instance, consider two atoms closely located. If they interact making a chemical bond, then both atoms have high electronegativity. Otherwise, atoms will not relate at all. Interestingly,



**Fig. 2.4** Tendency of electronegativity in the periodic table

**Table 2.1** Electronegativity values of atoms related to chemical organic compounds

Element	Electronegativity (Pauling scale)
<i>H</i>	2.1
<i>C</i>	2.5
<i>O</i>	3.5
<i>N</i>	3.0
<i>P</i>	2.1
<i>S</i>	2.5
<i>F</i>	4.0
<i>Cl</i>	3.0
<i>Br</i>	2.8
<i>I</i>	2.6
<i>At</i>	2.2

elements in the periodic table are arranged so that electronegativity increases from left to right and from top to bottom, except for the hydrogen atom that has similar electronegativity as atoms related to organic compounds. Figure 2.4 shows tendency of electronegativity in the periodic table. In addition, electronegativity values of the set of atoms related to organic compounds [2, 3] are also shown in Table 2.1.

Electronegativity is measured using the Pauling scale. It represents the absence of electronegativity with a zero-value and higher values represent higher electronegativity. For example from Table 2.1, hydrogen and astatine elements have smaller

electronegativity than fluorine which has the highest electronegativity even in the whole periodic table.

Moreover, electronegativity is useful when classifying chemical bondings. If the difference in electronegativity is less than 0.5 in the Pauling scale, then the chemical bonding is considered as covalent bond. If the difference in electronegativity is between 0.5 and 1.7, then it is a polar covalent bond (see Sect. 2.3). Finally, if the difference in electronegativity is greater than 1.7, then it is an ionic interaction.

### 2.2.2.2 Quantum Chemistry Principles

As mentioned previously, the ground-state principle assures energy minimization in chemical structures [1, 8]. However, three important quantum chemistry principles need to be stated before introducing ground-state formally. These quantum chemistry principles refer to theoretical observations that regulate chemical interactions among atoms.

**Aufbau Principle.** This principle states that electrons must fill lowest energy shells first. As an exception, electrons in  $d$  orbital have more stability when this orbital is half filled or full filled. Thus, one electron from the above  $s$  orbital is placed on the  $d$  orbital.

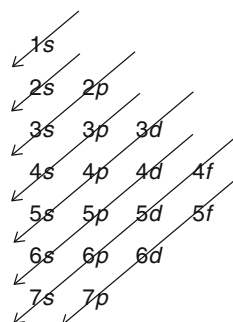
**Pauli exclusion.** This principle states that a pair of electrons in an orbital have to have opposite spins.

**Hund's rule.** It states that filling orbitals with electrons, these must not be in pairs on orbitals until each orbital contains one electron except when filling  $s$  orbitals.

Figure 2.5 shows the diagram for filling electrons in order to reach a ground-state in atoms [1, 8]. The arrows mean the path for picking up orbitals in order to filling them. Notice that the above three quantum chemistry rules must be satisfied.

*Example 2.1* Determine the ground-state electron configuration of: (a) the carbon atom, and (b) the copper atom.

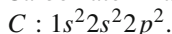
**Fig. 2.5** Diagram model for writing the ground-state electron configuration of atoms



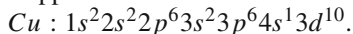


**Solution 2.1** Using Fig. 2.5 and the atomic number of each atom, the ground-state electron configuration is:

- (a) Carbon atom has atomic number six, thus six electrons are needed:



- (b) Copper atom has atomic number 29, thus 29 electrons are needed:



### 2.2.2.3 Ground-State Principle

Structures of chemical organic compounds preserve stability while minimizing energy. In practice, electrons have infinite number of configurations for each atom, and for each electron configuration it has an specific energy level. The electron configuration that has the minimum energy level is named ground-state [8]. Other electron configuration different from the ground-state is called excited-state. In organic chemistry, the ground-state electron configuration is considered for all chemical structures because it aims to study and understand physical and chemical properties.

On the other hand, ground-state has theoretical applications in energy minimization and chemical bonding. For instance, noble gases are the only elements with the minimum energies for each shell. It means that noble gases have filled full with electrons in the outer shell. Thus, atoms tend to fill the outer shell with all possible valence electrons. In organic chemistry, this rule is called the octet rule. In general, not all atoms claim for the rule, but in organic chemistry it is perfectly possible.

### 2.2.2.4 Lewis Dot Structure

A visual interpretation of ground-state, chemical bonding and electronegativity concepts all together, is the so-called Lewis dot structure. This diagram considers the chemical symbol of a given atom and some dots around it representing the valence electrons of that atom. Thus, sharing, gaining or losing electrons are seen explicitly. Figure 2.6 shows the Lewis dot structure of a carbon atom and the Lewis dot structure of the interaction between carbon and hydrogen atoms.



**Fig. 2.6** Examples of Lewis dot structures. (*left*) Diagram of carbon atom. (*right*) Diagram of interaction between carbon and hydrogen atoms

### 2.2.2.5 Chemical Balance Interaction

After atoms find ground-state electron configuration and molecules are formed via the octet-rule, another chemical interaction can be applied to minimize energy in structures. This is referring to the chemical balance theory [5, 8, 10]. Notice that it does not use atomic interactions.

In fact, chemical balance interaction determines different ways to mix two or more substances, e.g. molecules or compounds, by reacting and forming products, i.e. new compounds. In the simplest form, compounds might be determined as a linear mixture of substances in definite ratios. To this end, these ratios are named stoichiometric coefficients. In fact, if optimal stoichiometric coefficients were found, then chemical balance interaction can be viewed as an energy stabilization process. In chemistry, these structures are called mixtures.

## 2.3 Covalent Bonding

In Sect. 2.2.1.3, covalent bonds were defined. Since, they are important to organic chemistry, this section introduces the classification and an accepted chemical model for covalent bonds.

Rewriting, covalent bonds appear when two nonmetal atoms are sharing electrons of their outer shells because they cannot lose or gain electrons. In general, chemical interactions of two atoms with difference in electronegativity less than 1.7 in Pauling scale, are considered covalent bonds. An usual classification of covalent bonds are the following:

**Polar covalent bonds.** It appears when two different atoms are interacting, e.g. in  $C - H$  interaction.

**Nonpolar covalent bonds.** It appears when two similar atoms are interacting, e.g. in  $C - C$  interaction.

Below, there is a description of an accepted model of covalent bonds. In particular, it introduces the empirical model and two important parameters which are: the length and the minimum energy of bond.

### 2.3.1 Characterization of Covalent Bonds

In organic chemistry, the model of chemical covalent bonds refers to a mathematical expression that characterizes the chemical covalent bond between two atoms [5, 8]. In fact, this model relates the energy of bond and the interatomic distance. For instance, the energy of bond is the value of energy necessary to break the atomic bond; while the interatomic distance is the length between the nuclei of the two atoms participating in the chemical interaction. Additionally, the notion of covalent bonds between atoms

can be extended to covalent bonds between molecules, relating the energy of bond and the intermolecular distance which it refers to the interatomic distance of the two atoms located on distinct molecules participating in the interaction.

Without loss of generalization, interatomic distances are considered following [8]. On one hand, if the interatomic distance is too large, there is no chemical bond between atoms; thus, the energy of bond is equal to zero. On the other hand, let  $E_{attraction}$  be the energy related to the attraction force between electrons of one atom and the nucleus of the other which it increases rapidly when the distance is short. However, if atoms are too close, a repulsive force appears due to the electrons of both atoms and the energy associated to this force, let say  $E_{repulsion}$ , increases negatively. Then, the sum of both energies  $E_{attraction}$  and  $E_{repulsion}$  gets the total energy of bond  $E_{bond}$  as (2.1):

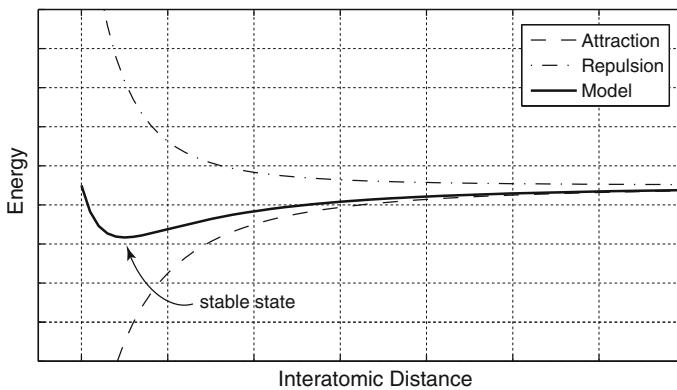
$$E_{bond} = -E_{attraction} + E_{repulsion} \quad (2.1)$$

In fact, the empirical model of chemical covalent bond (2.1) [8] can be rewritten in terms of the interatomic distance as expressed in (2.2):

$$E_{bond} = -\frac{A}{r^m} + \frac{B}{r^n}, \quad (m < n) \quad (2.2)$$

Where,  $A$  and  $B$  are constants related to the charge of atoms,  $r$  is the interatomic distance, and  $m, n$  are two positive empirical coefficients defining the attractive and repulsive forces, typically  $n \approx 12$  and  $m \geq 6$ . Figure 2.7 shows the relationship between  $E_{attraction}$  and  $E_{repulsion}$ .

Actually, two interesting parameters of covalent bonds are the length of bond and the minimum energy, and one parameter for specific nonpolar covalent bonds is called the order of bond:



**Fig. 2.7** Empirical model of chemical covalent bonds

**Length of bond.** It is the measurement of interatomic or intermolecular distance where the minimum energy of bond is reached.

**Minimum energy of bond.** It is the minimum energy required to break the bond, and it also represents the most stable state of chemical covalent bond.

**Order of bond.** (Nonpolar covalent bonds) It is the number of pairs of electrons shared in the covalent bond. While the order of bond increases, the covalent bond is physically stronger and more stable. Orders are:

**Simple bonds.** One pair of electrons are shared.

**Double bonds.** Two pairs of electrons are shared.

**Triple bonds.** Triple pairs of electrons are shared.

## 2.4 Energy in Organic Compounds

Energy is an important concept concerning into physics, chemistry, thermodynamics and generally in engineering. It can be defined as the ability of a system to do work. Referring to organic compounds, chemical energy is the responsible of structural transformation, combustion, electricity due to nuclear fission, batteries, etc.

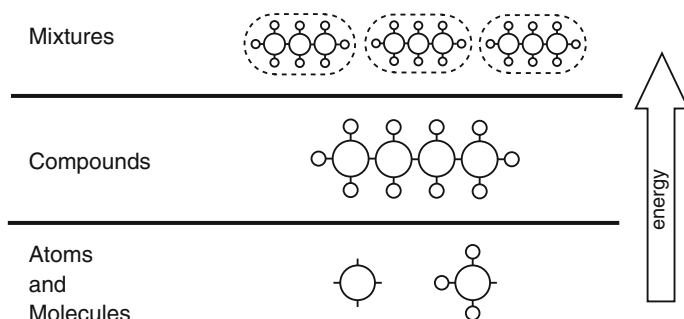
Typically, energy is classified into kinetic and potential energies. Roughly speaking, kinetic energy is the one used when any mass is in movement while potential energy is referred to as stored energy. Considering the latter, potential energy determines stability in chemical structures. If potential energy is low, structures are stable. If potential energy increases, chemical structures are unstable. Since potential energy could transform it to kinetic energy, the higher the potential energy is, the greater motion of chemical structures is, assuming rearranging in geometric structures of atoms, molecules and compounds. Thus, energy minimization refers to chemical structural stability.

In that sense, organic compounds have some strategies to minimize energy in their chemical structures, summarized in the following energy level scheme. Finally, three measurements of energy in thermodynamics are introduced.

### 2.4.1 Energy Level Scheme

In this section, it is proposed a model of energy minimization in chemical structures named the energy level scheme. In fact, this is a synthesis of concepts of quantum chemical structures, molecular formation and mixture formation.

Stability in organic compounds comes from the fact that every structural unit claims for energy minimization. Then, three levels of energy are considered. The first level of energy minimization refers to the ground-state electron configuration. Before any atom interact among others, atoms tend to minimize energy following



**Fig. 2.8** Representation of the energy level scheme

quantum chemical structures (see Sect. 2.2.2.2). In addition, since atoms aim to hold the octet-rule, they interact among them via chemical bonds forming molecules.

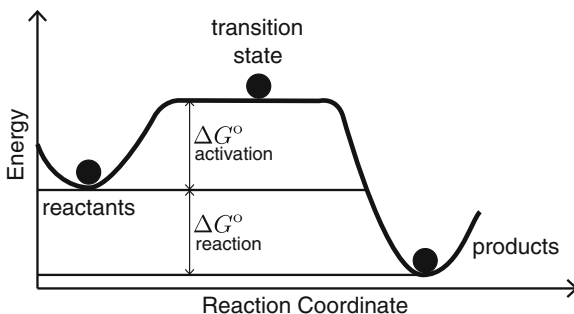
The next level of energy minimization considers chemical reactions on molecules to create compounds. These compounds are made of different molecules but interaction of them needs minimizing energy to conform bonds. In particular, these interactions release energy in structures by breaking and making bonds. Finally, the last level of energy minimization is presented in chemical balance interaction while creating mixtures of molecules or compounds.

As notice, atoms are more stable than molecules, molecules are more stable than compounds, and the latter are more stable than mixtures. Figure 2.8 represents visually this energy level scheme. It concludes that stability is preserved easily in the bottom level and structures are more unstable at the top level.

### 2.4.2 Measures of Energy

In thermodynamics—a branch of physics which describes the relationship between heat and work, changes in temperature, and transformation of energy—, transference and conversion of energy in chemical reactions are studied [1, 4]. Actually, three important thermodynamic properties are considered to measure energy in chemical reactions: enthalpy, Gibbs free energy, and entropy. In practice these properties cannot be measured directly to the system, thus the difference of them are useful, as mentioned later.

Consider a chemical reaction from reactants ( $R$ ) to products ( $P$ ) as depicted in Fig. 2.9. At the beginning, reactants have some energy and at a given time a chemical reaction is produced and the products have less energy than reactants. Visually, this is known as reaction coordinate diagram.



**Fig. 2.9** Example of a reaction coordinate diagram

### 2.4.2.1 Enthalpy

Enthalpy  $H$  is a thermodynamic property of chemical bonds [6]. In practice, the energy involved in these bonds is directly related to the chemical energy at constant pressure. Thus enthalpy can be measured using the heat in reaction. When computing the enthalpy in chemical reactions, Hess' law [6] states that enthalpy of a reaction is independent of the pathway between the initial and final states, then the heat of reaction <sup>1</sup>  $\Delta H^\circ$  is used instead of  $H$ , defined as (2.3); where,  $H_i^\circ$  is the initial enthalpy (e.g. energy of reactants) and  $H_f^\circ$  is the final enthalpy (e.g. energy of products). In laboratory, the heat  $Q$  measured with a calorimeter is equal to  $\Delta H$  such that (2.4) holds.

$$\Delta H^\circ = H_f^\circ - H_i^\circ \quad (2.3)$$

$$\Delta H^\circ = Q \quad (2.4)$$

In organic chemistry, several enthalpies of chemical bonds and molecules are already obtained. Table 2.2 summarizes enthalpies of chemical bonds related to important atomic interactions in organic compounds [4, 6, 8, 9].

Finally, heat of reaction determine if the reaction releases heat known as exothermic ( $\Delta H^\circ < 0$ ) or absorbs heat known as endothermic ( $\Delta H^\circ > 0$ ).

**Table 2.2** List of enthalpies of chemical bonds in organic compounds

Chemical bond	Enthalpy (kJ/mol)
$C - C$	350
$C - H$	415
$C = C$	611
$C \equiv C$	837

<sup>1</sup> The superscript ( $^\circ$ ) means that the property is measured at standard states of 298 K in temperature and 1 atm in pressure.

### 2.4.2.2 Gibbs Free Energy

The Gibbs free energy  $G$  is another thermodynamic property of chemical reactions that measures the velocity (rate) of reaction and its equilibrium [7]. At standard states, the change of Gibbs free energy  $\Delta G^\circ$  is related to the equilibrium constant  $K_{eq}$  as (2.5); where,  $R$  is the gas constant ( $8.314 \text{ J/mol} \cdot \text{K}$ ), and  $T$  is the temperature. If  $\Delta G^\circ < 0$  refers to an spontaneous reaction. Otherwise, reactions need external energy to produce it.

$$\Delta G^\circ = -RT \ln(K_{eq}) \quad (2.5)$$

Interestingly, enthalpy, entropy and Gibbs free energy are expressed together in the Gibbs-Helmholtz equation as (2.6); where,  $T$  is temperature,  $\Delta G^\circ$  is the change in Gibbs free energy,  $\Delta H^\circ$  is heat of reaction, and  $\Delta S^\circ$  is the change in entropy.

$$\Delta G^\circ = \Delta H^\circ - T \Delta S^\circ \quad (2.6)$$

### 2.4.2.3 Entropy

Entropy  $S$  is the measurement of the number of processes or possible conformations in chemical reactions [7]. Roughly speaking, entropy measures disorder in reactions. It is an statistical property associated to stability which it is associated to the second law of thermodynamics that states stable systems are those with maximum entropy. For instance, in standard states, if the change in entropy  $\Delta S^\circ > 0$ , then the system is more stable; and if the change in entropy  $\Delta S^\circ < 0$ , then the system is more unstable. This behavior is also observed in (2.6).

In practice, the change in entropy is calculated with (2.6) because there are no instruments to measure it directly in the system.

## 2.5 Classification of Organic Compounds

As discussed previously, chemical organic compounds are based on their own functional group (see Sect. 2.2.1.2). In fact, the most studied organic compounds are [4]: hydrocarbons, alcohols, amines, aldehydes, ketones, carboxylic acids, polymers, carbohydrates, lipids, amino acids, proteins, and nucleic acids. Following, there is a brief description of each type of compound.

### 2.5.1 Hydrocarbons

Hydrocarbons are the simplest organic compounds with functional group  $CH$  [10]. Hydrocarbons are classified as alkanes, alkenes and alkynes, depending on the order of bonds among carbon atoms of their functional group.

On one hand, alkanes are the simplest hydrocarbons formed by one polar covalent bond between two carbon atoms [10]. The general formula can be expressed as  $C_nH_{2n+2}$ , in which  $n$  is the number of carbon atoms in the molecule. Structural isomers are the different forms that alkanes can be expressed in terms of the topology of the molecules with the same number of elements. Structural isomers have particular physical and chemical properties.

Another type of hydrocarbons is the cyclic hydrocarbons in which carbons are ring-shaped bonded [10]. If all carbons in cyclic hydrocarbons are bonded with hydrogen fulfilling the octet rule, they are called cycloalkanes. In nature, the most abundant are cyclopentane and cyclohexenes.

When alkanes and cycloalkanes have low molecular weight tend to be gases and when it grows its molecular weight they are solids. This depends on the intramolecular forces and the melting and boiling points, where they become smaller as the dispersion forces become weak. The average density of alkanes is 0.8 g/ml, so they float in water [4]. Also, the more compact isomers (fewer branches) have a boiling point higher than the highly branched isomers. These organic compounds are more stable by strong  $CH$  bonds, but may react to form oxygen and oxidation. This oxidation can release heat that can be used as an energy source. Mainly, they come from fossil fuels.

Other types of hydrocarbons are alkenes and alkynes. Alkenes are unsaturated hydrocarbons having carbon atoms with double bond and alkynes are those with carbon atoms of triple bond. Also, the arenes are the functional groups formed by a ring of carbon with double bond. In general, they share the same physical and chemical properties of alkanes, but are not soluble in water, only on themselves. The most common processes in nature are the formation of  $CH$  skeletons that allow biodiversity, mainly in plants, where the structures are iterative and the ramifications are taken for enzymatic reactions. If any of the hydrogen atoms of an alkane is removed is known as alkyl and if one-hydrogen atom is replaced by a halogen is known as halo alkanes.

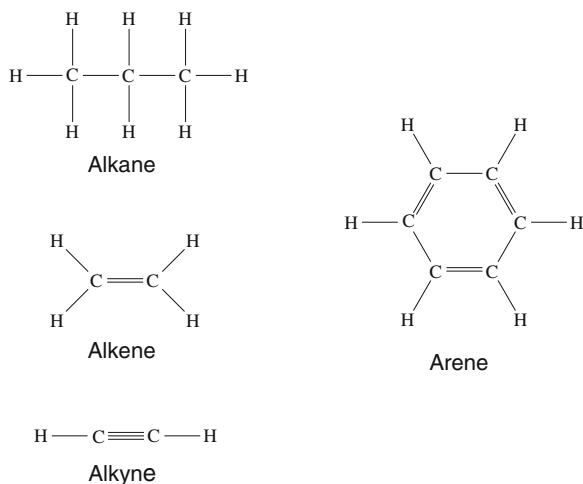
Figure 2.10 shows the difference among alkanes, alkenes, alkynes and arenes.

### 2.5.2 Alcohols, Ethers, and Thiols

On one hand, alcohols [4] are considered the central organic compounds because they can be transformed in other organic compounds or can be expressed as a product of reactions of other compounds. Their functional group is the hydroxyl  $-OH$  that is bonded to a carbon atom. In general, alcohols are more soluble in water than hydrocarbons since their molecular weight comes to grow. In addition, alcohols can form weak acids in presence of water; and in presence of strong acids, alcohols can form weak bases. Several compounds that alcohols can be converted are alkyl halides, alkenes, aldehydes, and carboxylic acids, among others.

On the other hand, ethers [4] have a functional group with oxygen bonded to two-hybrid carbon atoms  $sp^3$ . They are more soluble in water than hydrocarbons





**Fig. 2.10** Different types of hydrocarbons

because oxygen may form hydrogen bonds (weaker bond between a hydrogen and an electronegative element). In fact, ethers are very stable as hydrocarbons and they cannot react with the majority of organic compounds. Actually, ethers can help to chemical reactions in other organic compounds.

At last, thiols [4] are organic compounds with sulfhydryl  $-SH$  as functional group. Physically, they cannot form hydrogen bonds; thus, the boiling point of thiols is lower than alcohols or ethers. Moreover, thiols may not be too soluble in water.

### 2.5.3 Amines

The functional group of amines is the *amino*, a compound formed with nitrogen and one, two, or three groups of carbon atoms [3, 4]. Depending on the ammonia, amines can be classified as primary amines if its ammonia has one-hydrogen atom replaced; secondary amines if its ammonia has two-hydrogen atoms replaced; or tertiary amines if its ammonia has three-hydrogen atoms replaced. In fact, amines can present hydrogen bonds with nitrogen atoms. The greater the molecular weight amines present, the less soluble in water they can be.

### 2.5.4 Aldehydes, Ketones, and Carboxylic Acids

First, aldehydes [3] have a carbonyl functional group  $C=O$ , and a union of one or two hydrogen atoms. Ketones [3] have the same carbonyl functional group union

with two-carbon atoms. In general, the boiling point of aldehydes and ketones is higher than the boiling point of nonpolar compounds. Aldehydes can react in order to form carboxyl acids because they are the one of the easiest compounds that can oxidize. In contrast, ketones cannot oxidize easily.

On the other hand, carboxylic acids [3] have the carboxyl functional group  $-CO_2H$ . This functional group is a hybrid between a carbonyl and a hydroxyl. In reactions, carboxyl acids can be converted into acid chlorides, esters and amides. Because carboxyl acids have oxygen and hydrogen atoms, they are quite stables and can form hydrogen bonds. In comparison with aldehydes, ketones or amines, carboxyl acids have large boiling points.

### 2.5.5 Polymers

In organic compounds, polymers are molecules of long chains formed by monomers (simplest organic compound) bonded [3, 4]. In general, polymers have different structures, the most common are: linear, branched, comb-shaped, ladder, star, cross-linked network, and dendritic. The properties of polymers depend on the size and topology of the molecules. Physical properties of polymers are related to resistance, elasticity, and so forth. In general, monomers used in polymers are iteratively repeated through the whole network, and relations are done by covalent bonds.

There exist two processes of polymer synthesis. Step-growth polymerization is a laboratory synthetic process in which monomers are added to the chain one at a time. Since, polymerization is the process in which small molecules are added to the chain in one chemical reaction without loss of atoms. The most important polymer structures are polyamides, polyesters, polycarbonates, polyurethanes, and epoxies.

### 2.5.6 Carbohydrates, Lipids, Amino Acids, and Proteins

These are considered as biomolecules and they are associated to a chemical function [1]. In that context, carbohydrates [1] are compounds that can store energy, form part of structural tissues, and they are part of nucleic acids. The majority of carbohydrates are based on the formula  $C_n(H_2O)_m$ .

Lipids [1] are organic compounds typically known as the energy source of living beings. In contrast, amino acids [1] are organic compounds formed with a carboxyl and an amino, used in the transportation of enzymes. Alpha-amino acids are monomers of proteins.

Finally, proteins [1] are organic compounds with one or more chains of polypeptides, macromolecules containing ten or more amino acids joined together with peptide bonds. In general, proteins are the structural basis of organisms, the growth regulators, the transportation of other molecules, etc.

### 2.5.7 Nucleic Acids

Other biomolecules are the nucleic acids [1, 4]. They form the basis of information over the organization, maintenance, and regulation of cellular functions. This information is expressed in genes via deoxyribonucleic acids (DNA) translated by ribonucleic acids (RNA) in the synthesis of proteins. Roughly speaking, the structure of DNA is based on deoxyribose units and phosphate, in which simple bases of aromatic heterocyclic amines mate to them: adenine, guanine, thiamine, and cytosine. The entire structure has two helices. Observations summarized the following:

- Composition of bases in any organism is the same in every cells of the organism, and it is unique to it.
- Molar percentages of adenine and thiamine are equal.
- Molar percentages of guanine and cytosine are equal, too.
- Molar percentages of purine bases (adenine and guanine) and the pyrimidine bases (cytosine and thiamine) are equal.
- In comparison to DNA, RNA is based in one structure in which uracil and cytosine are bases rather than thiamine and cytosine.

## 2.6 Organic Compounds as Inspiration

As reviewed, organic compounds are represented physically and chemically. However, these representations are intimately related because structures are conformed under chemical rules. In addition, these compounds aim to reach stability via energy minimization. In fact, this point of view inspired artificial organic networks. Thus, this section introduces the motivation of that inspiration and the characteristics studied.

### 2.6.1 Motivation

When looking at nature, and more specifically at the structure of matter, some characteristics of chemical compounds are rapidly noticeable. For instance, just around eleven elements can derived in more than twenty millions of different organic compounds. In addition, compounds are made of other simple molecules that it can be described as organized units. Also, this organization is based on chemical rules that are applied over and over again from bottom to top in the energy level scheme. But the must important observation is that chemical structures look for stabilization via energy minimization. Thus, organic compounds are made of minimal resources and optimal ways to do that.

Actually, notice that the relationship of atoms makes possible molecular units. Different atoms and different arrangements of those make different molecules. Notice

that the differentiation of molecules may be observable from their physical and chemical properties. In that sense, physical properties may refer to the structure of the molecule while chemical features may refer to the behavior of that molecule. Thus, molecules can be seen as basic units of information characterized by the atoms in the inside. Moreover, molecules might be seen as encapsulation and potential inheritance of information. However, relationships among atoms cannot be performed without two possible interactions: chemical bonds and chemical reactions. The first interaction forms basic and complex molecules, and the second one forms mixtures of molecules.

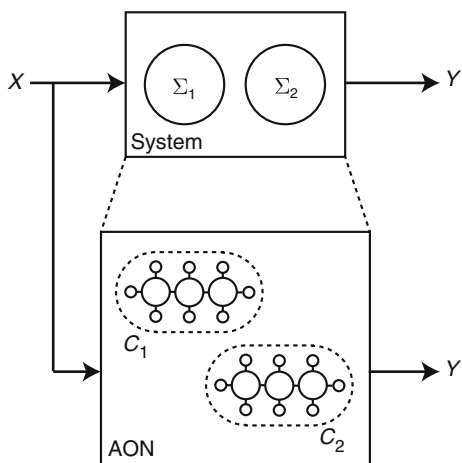
### 2.6.2 Characteristics

From the above motivation, systems inspired on chemical organic compounds will have the characteristics described below. In Fig. 2.11 is shown a diagram explaining these characteristics assuming a system inspired on chemical organic compounds.

#### 2.6.2.1 Structural and Behavioral Properties

On one hand, structural properties refer to units or subsystems with specific properties. For instance, these units are molecules while specific properties are atoms. On the other hand, behavioral properties refer to functions or processes inside units. These processes are chemical interactions and chemical behaviors of compounds.

**Fig. 2.11** Example of a system inspired on chemical organic compounds



### 2.6.2.2 Encapsulation

Structural units with processes can be encapsulated. Thus, information of subsystems can be easily clustered. In fact, inheritance and organization are derived from this characteristic.

### 2.6.2.3 Inheritance

Consider a given, known system that is inspired on chemical organic compounds. If another, unknown system has similar behavior to the given one; then, structural units from the known system might be inherited to the unknown system. This characteristic comes from the encapsulation property.

### 2.6.2.4 Organization

Since structural units encapsulate information, these can be organized from basic to complex units. Basic units are the ones that have elemental information, e.g. with low energy, and complex units are made of combination of basic units, e.g. with high energy. The energy level scheme can be used in order to organize information into molecular units, compound units and mixture units. For example, mixtures can contain several compounds, each one assimilating different characteristics of the whole system inspired on chemical organic compounds.

### 2.6.2.5 Mixing Properties

Organization can derive in mixing properties. As described previously, molecular units can be seen as pieces of a puzzle; thus molecules can chemically interact among them in order to create complex units as compounds or mixtures.

### 2.6.2.6 Stability

Since it is the central observation of organic compounds, stability is one of the most important characteristics of systems inspired on chemical organic compounds. Structural units, encapsulation, inheritance, mixing properties and organization are possible due to energy minimization. Structures of these kinds of systems will be made of minimal units, and optimality will be found. Thus, energy is an important property of systems inspired on chemical organic compounds. As explained before, chemical rules (i.e. Aufbau principle, Pauli exclusion and Hund's rule) help molecular structures to be stable since atoms and molecules are arranged suitably such that the overall structure has the minimum energy.

### 2.6.2.7 Robustness

The notion of the finite small set of atoms and the huge amount of different organic compounds characterizes systems inspired on chemical organic compounds in robustness. This characteristic can be seen as the power of finite set of parameters to model a large set of different systems.

## References

1. Bettelheim FA, Brown WH, Campbell MK, Farrell SO (2008) Introduction to general, organic and biochemistry. Cengage Learning, Belmont
2. Bhushan B (2007) Springer handbook of nanotechnology. Springer, Berlin
3. Brown TL, Lemay HE, Bursten BE, Murphy CJ, Woodward PM (2009) Chemistry: the central science. Pearson Education, Upper Saddle River
4. Brown WH, Foote CS, Iverson BL, Anslyn EV (2011) Organic chemistry. Cengage Learning, Belmont
5. Carey FA, Sundberg RJ (2007) Advanced organic chemistry: part A: structure and mechanisms. Springer, New York
6. Ganguly J (2009) Thermodynamics in earth and planetary sciences. Springer, Berlin
7. Greiner W, Neise L, Stocker H (1995) Thermodynamics and statistical mechanics. Springer, Berlin
8. Klein DR (2011) Organic chemistry. Wiley, Hoboken
9. Lide DR (2008) CRC handbook of chemistry and physics. Taylor and Francis, Boca Raton
10. Quinkert G, Egert E, Griesinger C (1996) Aspects of organic chemistry: structure. Wiley, New York

Artificial Organic Networks

Artificial Intelligence Based on Carbon Networks

Ponce Espinosa, H.E.; Ponce-Cruz, P.; Molina, A.

2014, XII, 228 p. 192 illus., 56 illus. in color. With online files/update., Hardcover

ISBN: 978-3-319-02471-4