



Organic Chemistry for Health and Life Sciences Handout 1.1

Atomic Structure and Bonding, Part 1

by Kevin M. Chevalier

***For pictures, please refer to the 1.1 Atomic Structure and Bonding Figures Sheet that accompanies this handout**



Organic chemistry is the study of compounds containing carbon. There are no differences between organic and inorganic compounds since their behaviors are similar regardless of their origin and no matter how complex they are. The only difference is that organic compounds contain **carbon**.

Carbon is a group 4A (14 in IUPAC System) element which means that it can share **four valence electrons** and form **four strong covalent bonds**.

Carbon can form diverse compounds ranging from simple to complex since it can bond to each other to form long chains and rings. (See Diagram 1A)

Organic compounds come from both living organisms and through synthesis (medicines, polymers, cosmetics, and other substances) in a laboratory.

Atomic Structure Review

Atoms consist of a dense, positively charged nucleus surrounded at a large distance by negatively charged electrons.

The atom's nucleus is composed of:

Protons- positively charged subatomic particles

Neutrons- electrically neutral subatomic particles

An atom is overall neutral meaning that the number of protons (positive) in the nucleus is the same as the number of electrons (negative) surrounding the nucleus.

Electron mass is negligible and circle the nucleus at a distance of 10^{-10} m
Nucleus is around 10^{-14} to 10^{-15} meters (m) in diameter.

Diameter of a typical atom is 200 picometers (pm) or 2×10^{-10} m.

Where 1 picometer (pm) = 10^{-12} meters (m)

Many organic chemists and biochemists also use the angstrom (Å) to express atomic distances.

Where $1 \text{ Å} = 100 \text{ pm} = 10^{-10} \text{ m}$

Atoms are described by their atomic number (Z) which tells you the number of protons (as well as electrons since their number is the same) it contains.

- For example, the atomic number for oxygen is 8. Therefore, it has 8 protons and 8 electrons.

The mass number (A) tells you the total number of protons and neutrons in the nucleus. Depending on the number of neutrons, atoms with the same atomic number can have different masses.

Atoms with the same atomic number and different numbers of neutrons are called isotopes.

- For example, let's take a look at carbon (since it is orgo after all!). Carbon's atomic number is 6. It has 6 protons, 6 neutrons, and 6 electrons. An isotope of carbon is Carbon-13 (^{13}C) which has 6 protons, 7 neutrons, and 6 electrons.

The atomic mass (atomic weight) of an element is the weighted average mass of an element's naturally occurring isotope (in atomic mass units).

Let's use our previous example for carbon and look at its two stable isotopes ^{12}C and ^{13}C . If the definition above looks confusing, take a look at the example and it should be easier to visualize and understand.

Mass Number	Atomic Weight	Percent Abundance
12	12.000	98.90%
13	13.0033	1.1%

If you want a refresher from general chemistry:

To calculate the average atomic weight of an element (for example, carbon):

Atomic weight = $\Sigma(\text{isotopic abundance}) \times (\text{isotopic mass})$

Carbon-12 (^{12}C): $(0.9890 \times 12 \text{ amu}) = 11.868 \text{ amu}$

Carbon-13 (^{13}C): $(0.011 \times 13.0033 \text{ amu}) = 0.143 \text{ amu}$

Add them together $(11.868 \text{ amu} + 0.143 \text{ amu}) = 12.011 \text{ amu}$ (take a look at carbon's mass number on the periodic table and it's the same)

Orbitals

A specific electron's behavior in an atom can be described by a **wave equation** which is a mathematical expression defining the electron's behavior in an atom. The solution of a wave equation is called a **wave function (orbital)**. It is represented as the Greek letter, psi (Ψ).

The square of the wave function (Ψ^2) defines the shape of an orbital. If you plot Ψ^2 in three-dimensional space, it will describe the volume of space around a nucleus that will most likely be occupied by an electron. We can visualize it from the diagrams (Diagrams 1B and 1C).

If you remember from general chemistry there are four types of orbitals (s, p, d, and f). The most common orbitals in organic chemistry and biochemistry are **s** and **p** and will be the ones focused on.

An orbital represents the space where an electron will occupy most of the time.

Shapes of orbitals (See Diagram 1B)

s: spherical with the nucleus at its center

p: dumbbell-shaped

d: four of the five d orbitals are cloverleaf-shaped; fifth d orbital is shaped like an elongated dumbbell with a doughnut around its middle

An atom's orbitals are organized into electron shell layers that increase in size and energy.

Each shell contains a different number and different types of orbitals. **Each orbital within a shell can hold two electrons.**

Subshells

s subshell: one orbital, holds two (2) electrons

p subshell: three orbitals, holds six (6) electrons

d subshell: five orbitals, holds ten (10) electrons

f subshell: seven orbitals, holds fourteen (14) electrons

If it's confusing, don't worry we'll break it down.

From general chemistry, we can divide the periodic table into different blocks (s block, p block, d block, f block). Elements are grouped in blocks based on the highest energy orbital filled by an electron.

S block

S block is composed of Groups 1 (1A) and 2 (2A) on the periodic table. Note that helium is in the s block ($1s^2$).

P block

P block is composed of Groups 13 through 18 (3A through 8A) except helium.

D block

D block is composed of the transition metals, Groups 3 through 12.

F block

F block is composed of the inner transition elements (lanthanide and actinide series).

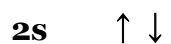
The first shell only has one 1s orbital. It holds a maximum of 2 electrons.

1st shell:



The second shell has one 2s orbital and three 2p orbitals. It holds a maximum of 8 electrons (2s holds two electrons, 2p holds six electrons).

2nd shell:



The third shell has one 3s orbital, three 3p orbitals, and five 3d orbitals. It holds a maximum of 18 electrons (3s holds two electrons, 3p holds six electrons, 3d holds ten electrons).

3rd shell:



The three p orbitals are mutually perpendicular, have a node that separates the two lobes, and have a dumbbell shape. The node is a region of zero electron density (the probability of finding an electron is zero). **(See Diagram 1C)**

The node separates the two lobes which have different algebraic signs (positive + and negative -) in the wave function. It doesn't refer to charge. It means that the positive lobe increases the electron density in its region while the negative lobe decreases

electron density in its region. This plays an important role in bonding when we look at molecular orbital theory.

In the next section, we will learn how to arrange an element's ground state configuration.

Electron configuration

Ground-state electron configuration is an atom's electron configuration (arrangement) at the lowest energy level.

There are three rules that help predict the electron's arrangement in an atom's shell and subshells:

Rule 1: From the aufbau principle, electrons occupy the lowest energy orbitals first starting with 1s.

The orbital energies increase starting from s, then to p, d, and f. After 3p, 4s comes between 3p and 3d. To visualize it, let's look at the chart.

1s -> 2s -> 2p -> 3s -> 3p -> 4s -> 3d -> 4p -> 5s -> 4d -> 5p -> 6s etc.

It might be confusing, but when you lay it down in chart form, it will make things easier.

1s	2s	3s	4s	5s	6s	7s
	2p	3p	4p	5p	6p	7p
		3d	4d	5d	6d	7d
			4f	5f	6f	7f

Draw a diagonal from the number on the left and move it to the upper right. It will match the arrows above the chart. 1s and 2s are the only ones in their diagonal, but when you start at 2p, its diagonal moves to 3s. The diagonal from 3p moves to 4s. Then the diagonal from 3d moves to 4p then 5s.

It's easier to visualize because some students get mixed up when the 4s comes between 3p and 3d.

Rule 2: Each orbital can have two electrons occupying it. Their spin has two orientations up ↑ and down ↓. According to the Pauli exclusion principle, the two electrons occupying an orbital must spin in opposite directions (the more detailed explanation goes into quantum mechanics, but this is the main point that you'll need to know).

Example: Helium, atomic number is 2. It's electron configuration is 1s²

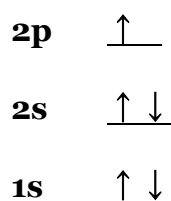
1s ↑↓

Rule 3: According to Hund's Rule, if there are two or more orbitals with the same energy (we'll begin to see this in the three p orbitals and the five d orbitals), one electron occupies the orbital (half filled) parallel to each other before you fill it with a second electron.

Let's take a look at an example to visualize it.

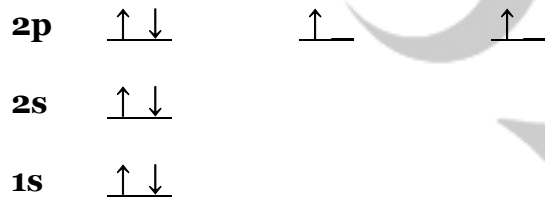
Example: Carbon, its atomic number is 6. Its electron configuration is therefore, $1s^2 2s^2 2p^2$

Using the rules that we learned from Rule 1 and 2, we write out its electron configuration. Then we apply Rule 3 to half fill the orbitals parallel to each other.



We can see from this that one electron half fills all of the orbitals before adding a second electron with an opposite spin. Let's take a look at oxygen now.

Example: Oxygen, atomic number 8. Electron configuration $1s^2 2s^2 2p^4$



From oxygen, we have filled the 2p orbitals first and then go back and fill the orbital with an electron of an opposite spin.

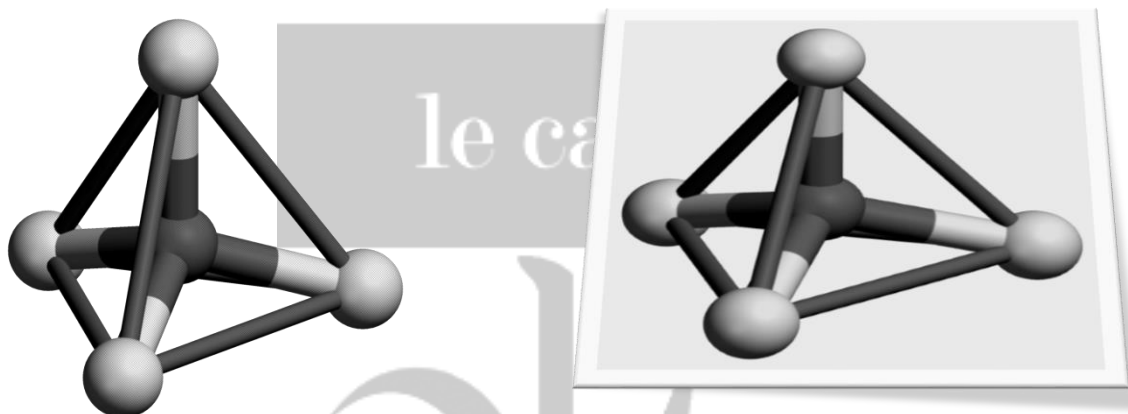
Chemical Bonding Theory

We previously learned that carbon is tetravalent (forms four bonds with elements to create stable compounds) as well as form bonds with each other to form longer chains.

August Kekulé and Archibald Couper independently proposed carbon's tetravalent nature (first part of the previous sentence) while Kekulé extended this to include carbon bonding with each other to form an extension of carbon atom chains (second part of the previous sentence).

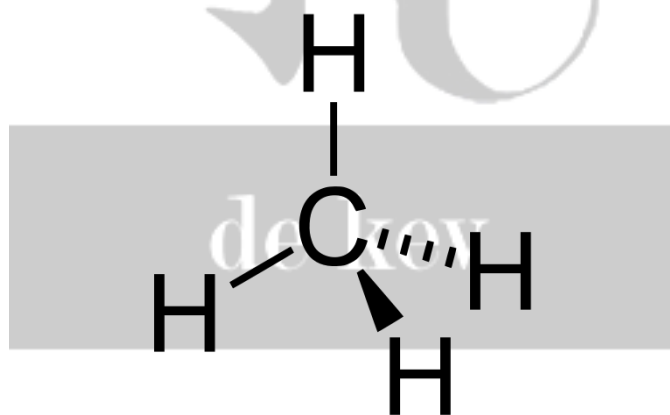
Chemistry moved from a two-dimensional view to a three dimensional view where the tetrahedral carbon was represented as a pyramid (tetrahedron) shape. It was proposed by Jacobus van't Hoff and Joseph Le Bel that the carbon molecules had specific directions in space rather than being situated in a random orientation.

van't Hoff then proposed that the four atoms which carbon is bonded to are located at the corners of the tetrahedron with carbon at its center. Let's take a closer look:



Two views of the tetrahedral carbon bonded to four hydrogens to form methane, CH_4 . If we situate it on the page's plane (picture to the right), we can see one bond jumping out of the page and other moving towards the back.

A modern representation of carbon's tetrahedral form which you will encounter in orgo:



Methane, CH_4

The solid line is on the plane on the page. The two carbon-hydrogen bonds are on the page's plane.

The thick wedged line jumps out of the page (out of the page's plane) toward the reader.

The dashed line represents the bond oriented toward the back of the page (receding toward the back of the page's plane), away from the reader.

Atoms bond together to form more stable compounds with lower energy. When a chemical bond is formed, energy in the form of heat is released. Likewise, energy is required to break a bond.

Simply speaking:

- Forming bonds = releases energy
- Breaking bonds = absorbs energy

We learned from general chemistry that an electron octet in an atom's valence shell (the outermost shell in an atom) gives it stability. This simply states that main group elements form bonds to have eight electrons in its outer shell so that they take on the electron configuration of the nearest noble gas.

If we look at the periodic table, carbon is in group 4A. It has four valence electrons in its outer shell so it will need to form four bonds by sharing with other atoms to take on noble gas configuration. The sharing of electrons to form a bond is called a covalent bond.

This differs from an ionic bond where atoms gain or lose electrons to bond together through electrostatic attraction. If we look at KCl (potassium chloride), potassium (K) is in Group 1A so it needs to lose an electron to form a cation and reach noble gas configuration while chlorine (Cl) is in Group 7A and needs to gain an electron to reach noble gas configuration.

Two ways to show covalent bonds (See Diagram 1D):

- Electron-dot structures (Lewis structures)- valence shell electrons are represented as dots
- Line-bond structures (Kekulé structures)- the two electrons in a covalent bond are represented as a solid line drawn between the atoms

Please refer to the table for a summary of atoms and how they form covalent bonds.

	Group Number	Valence Electrons	Number of electrons needed to reach noble-gas configuration	Number of bonds it can form	Number of lone pairs
Hydrogen	1A (1)	1	1	1	0
Carbon	4A (14)	4	4	4	0
Nitrogen	5A (15)	5	3	3	1
Oxygen	6A (16)	6	2	2	2
Fluorine, Chlorine, Bromine, Iodine	7A (17)	7	1	1	3

The valence electrons that not shared (not forming a bond) are called **lone-pair electrons**. In line-bond structures, the lone-pairs are not usually drawn, but are kept in mind. Please see Diagram 1E in the diagram handout to visualize the chart in action.

In the next handout, we will cover valence bond theory and hybridization.

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