Organic Chemistry for Chemical Engineers

Dr. Sompop Sanngraj

Introduction

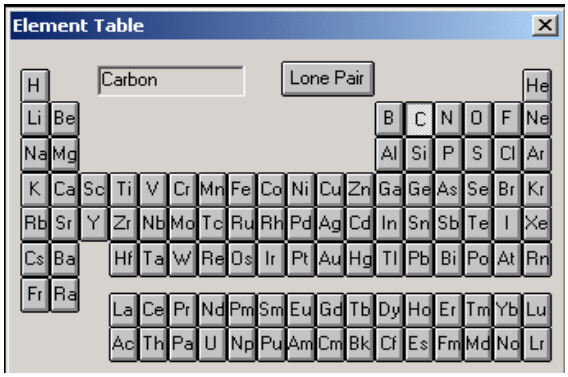
Organic chemistry: the study of carbon compounds.

An understanding of organic chemistry must begin with an understanding of molecular structure.

“Structure is the key to everything in chemistry (Atkins and Carey, 2002)”.

Chemistry Background

Element: is a simple, elementary substance. An element cannot be separated, or decomposed into simpler substances



Each element is made up of very small entities called atoms.

Atomic Symbols

- Each element is assigned a unique symbol.
- Each is 1-2 letters and the first is capitalized.
- Symbol may not match the name - often had a different name to start with.

arsenic	As	potassium	K
barium	Ba	nickel	Ni
carbon	C	nitrogen	N
chlorine	Cl	oxygen	O
hydrogen	H	radon	Rn
helium	He	titanium	Ti
gold	Au	uranium	U

Periodic Table: by increasing atomic no.

- Main group (1A-8A, A is often omitted) → Representative elements
- Subgroup (1B-8B) → Transition elements
- Lanthanide series (rare-earth elements)
- Actinide series (heavy rare-earth elements)

*Remark: The lanthanides and actinides together are called the inner transition elements)

Metals: generally solid, shiny in appearance, electrically conducting, and malleable

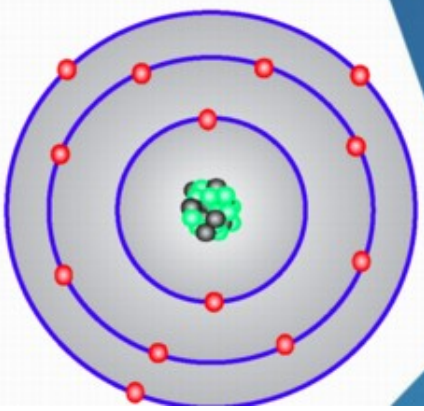
Nonmetals: generally liquid or gas, dull appearance, and not malleable

Metalloids: elements with properties intermediate between those of metals and nonmetals

Simple model of the atom

Commonly called the Bohr model

- Electrons moved around nucleus in orbitals
- Electrons are found only in orbitals.
- Orbitals have fixed energy values called quantum levels.

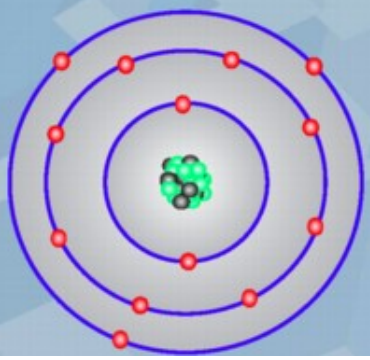


The Bohr Model

Atoms don't really look like this.

We know that the model is incorrect but it is good enough to help us understand many important concepts.

Niels Bohr



Structure of the atom

Atoms have a specific arrangement.

Nucleus

Small, dense, positive charge in the center of an atom that contains protons & neutrons.

Electrons

Surround the nucleus. Diffuse region of negative charge.

Nucleus is a very small part of an atom.

If it was the size of a marble, the atom would fill a football stadium.

Atom

The smallest unit of an element that retains its chemical properties.

Atoms can be split into smaller parts.

Atomic structure

Name	Symbol	Charge	AMU	grams
electron	e^-	-1	5.4×10^{-4}	9.11×10^{-28}
proton	p	+1	1.0	1.67×10^{-24}
neutron	n	0	1.0	1.67×10^{-24}

Atomic number: is equal to the number of protons in the nucleus of the atom.

Atomic mass: is the average mass of the atom.

Atomic mass is usually expressed using a very small unit called the atomic mass unit, amu (also called the dalton).

The amu is defined as 1/12 of the mass of the most common isotope of carbon (C-12).

Atom Nucleus: Proton + Neutron → has essentially all of the mass, but occupies virtually none of the volume, of the atom

Electron Cloud: Electron → occupies most of the volume of the atom

Isotope: the same no. of protons but different no. of neutrons in their nuclei

Isotopes

Isotopes Atoms of the same element but having different masses.

Each isotope has a different number of neutrons

Isotopes of hydrogen $^{1}_{1}H$ $^{2}_{1}H$ $^{3}_{1}H$

Isotopes of carbon $^{12}_{6}C$ $^{13}_{6}C$ $^{14}_{6}C$

Isotopes

Most elements occur in nature as a mixture of isotopes.

Element	# of stable isotopes
H	2
C	2
O	3
Fe	4
Sn	10

This is one reason why weights are not whole numbers. They are based on averages.

The atomic symbol

A - Atomic mass	- Total protons & neutrons
Z - Atomic number	- # of protons or electrons
C - Charge	- + or - values
# - Number	- # of atoms in a formula.

Formula

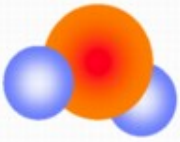
Formula are used to represent the elements in a compound.

- Lists the elements in a compound.
- Tells how many of each element there are.
- May also show how the elements are connected to each other.

H_2O - water
2 hydrogen
1 oxygen

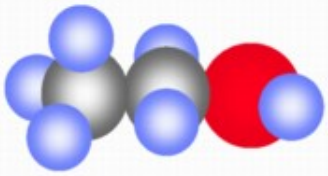
CH_3CH_2OH - ethyl alcohol
2 carbon, 6 hydrogen and 1 oxygen
(shows how atoms are arranged)

Molecular representations



H_2O - water

CH_3CH_2OH - ethyl alcohol



Masses of atoms and molecules

Atomic weight

- The average, relative mass of an atom in an element.

Atomic mass unit (amu)

- Arbitrary mass unit used for atoms.
- Relative to one type of carbon.

Molecular or formula mass

- The total mass for all atoms in a compound.

Molar masses

Once you know the weight of an atom, ion, or molecule, just remember:

Mass of one unit
- use AMU

Mass of one mole of units
- use g/mol

The numbers DON'T change -- just the units.

Another example

CH_3CH_2OH - ethyl alcohol

2 carbon	2 x	12.01 amu
6 hydrogen	6 x	1.008 amu
1 oxygen	1 x	16.00 amu
mass of molecule		46.02 amu
		46.02 g/mol

Molecular Mass: the average mass of all atoms of a compound

C_2H_4 = 2x12.0 amu+4x1.0 amu = 28.0 amu

The mass of 1 mole of C_2H_4 is 28 g

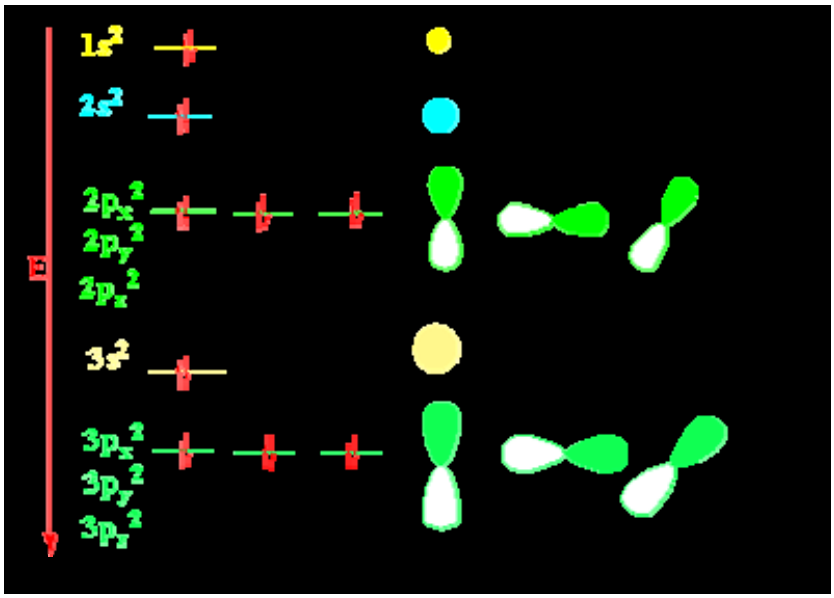
Chemical compound: a substance is formed by chemical bonds between atoms of two or more different elements.

"Periodicity in the properties of the elements is the result of the periodicity in the electronic configurations of their atoms"

-Orbital (2 electrons, spin up and down)
- Subshells (orbitals are grouped in sets)
  - s (1 orbital, 2 electrons)
  - p (3 orbitals, 6 electrons)
  - d (5 orbitals, 10 electrons)
  - f (7 orbitals, 14 electrons)
- Shells (subshells are grouped in sets)
  - K (1s subshell)
  - L (2s and 2p subshells)
  - M (3s, 3p and 3d subshells)

and so on

Energy levels and Orbitals



Electrons are arranged in different energy levels or shells.

The Electrons that are closer to the nuclei are lower in energy.

Each shell has sublevels (1,2,3, ..etc.) which have orbitals.

An orbital can hold a pair of electrons of opposite spins.

RULES GOVERNING THE ALLOWED COMBINATIONS OF QUANTUM NUMBERS

- The three quantum numbers (n, l, and m) that describe an orbital are integers.
- The principal quantum number (n) cannot be zero. The allowed values of n are therefore 1, 2, 3, 4, and so on.
- The angular quantum number (l) can be any integer between 0 and $n - 1$. If $n = 3$, for example, l can be either 0, 1, or 2.
- The magnetic quantum number (m) can be any integer between $-l$ and $+l$. If $l = 2$, m can be either -2, -1, 0, $+1$, or $+2$.

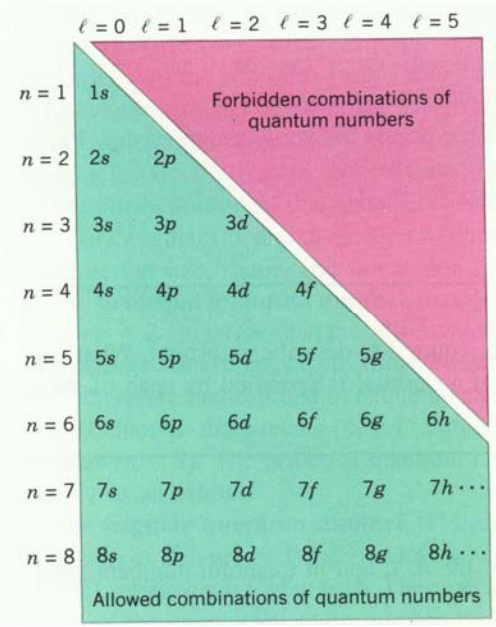


Figure 6.17 Only certain combinations of the principal (n) and angular (l) quantum numbers are allowed.

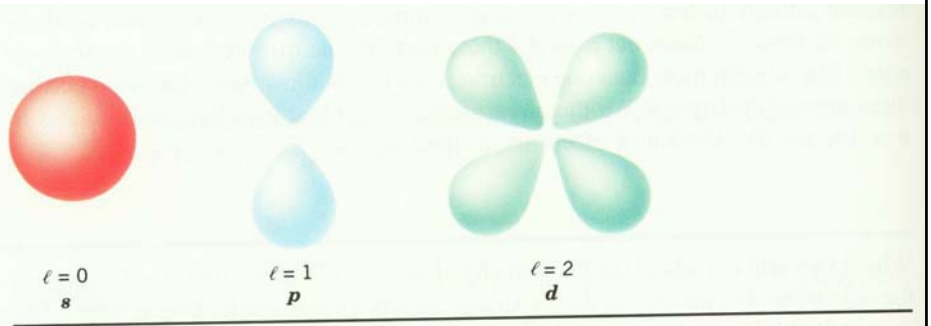


Figure 6.16 The angular quantum number specifies the shape of the orbital where electrons can be found. When $l = 0$, the orbital is spherical. When $l = 1$, the orbital is polar. When $l = 2$, the orbital typically has the shape of a cloverleaf.

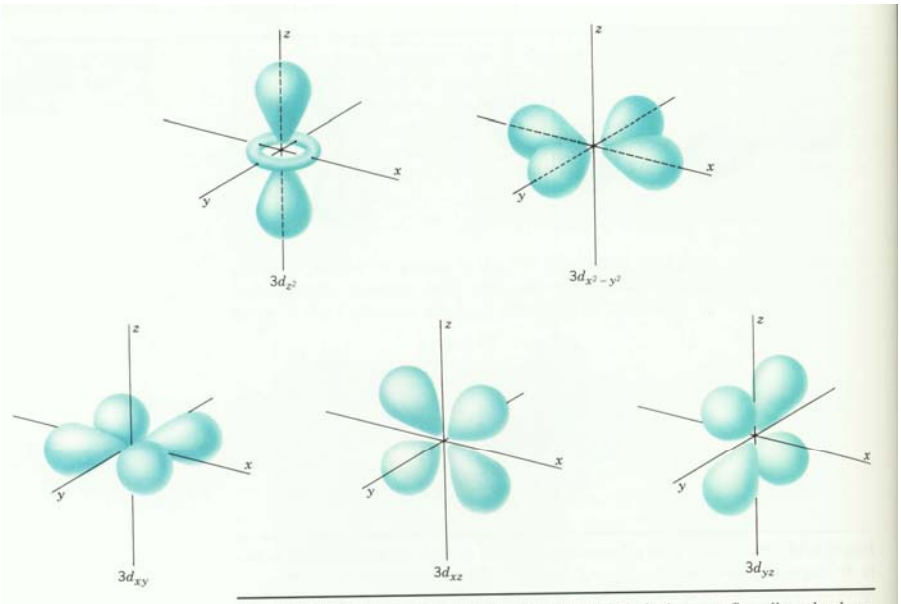


Figure 6.19 When the angular quantum number (l) is 2, there are five allowed values of the magnetic quantum number (m) corresponding to the five different orientations of these orbitals in space.

Figure 6.22 The energy of an orbital increases as either the principal quantum number (n) or the angular quantum number (l) becomes larger. The energy of an orbital in a given shell is therefore often higher than the energy of orbitals that are formally in a larger shell.

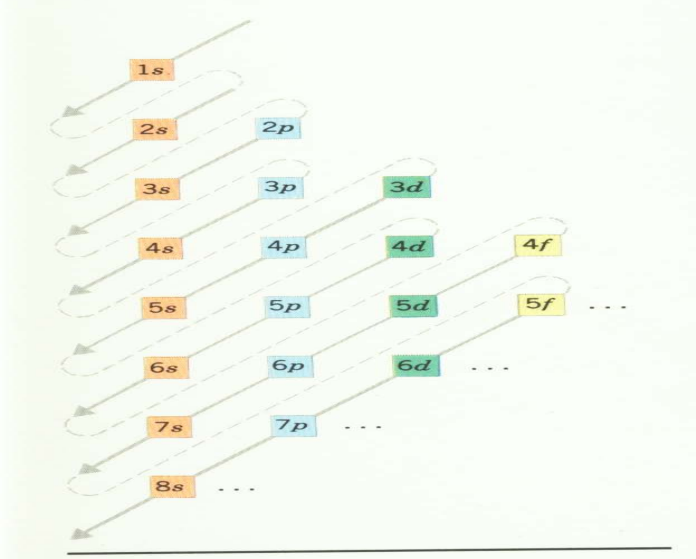


Figure 6.23 The order of increasing energy for atomic orbitals can be predicted by simply following the arrows in this diagram: $1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p$, and so on.

TABLE 6.4 Summary of Allowed Combinations of Quantum Numbers

n	l	m	Subshell Notation	Number of Orbitals in the Subshell	Number of Electrons Needed to Fill Subshell	
1	0	0	1*s*	1	2	total: 2
2	0	0	2*s*	1	2	
2	1	1,0,−1	2*p*	3	6	total: 8
3	0	0	3*s*	1	2	
3	1	1,0,−1	3*p*	3	6	
3	2	2,1,0,−1,−2	3*d*	5	10	total: 18
4	0	0	4*s*	1	2	
4	1	1,0,−1	4*p*	3	6	
4	2	2,1,0,−1,−2	4*d*	5	10	
4	3	3,2,1,0,−1,−2,−3	4*f*	7	14	total: 32

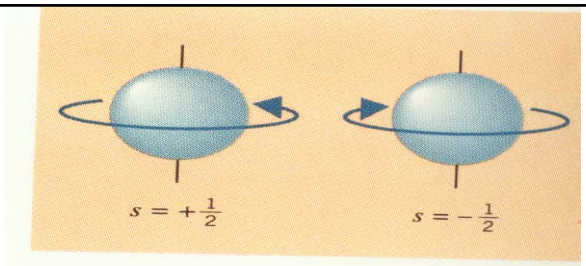


Figure 6.20 It takes three quantum numbers to describe an orbital. A fourth quantum number is then used to differentiate between the two electrons that can occupy an orbital. Because these electrons behave as if they are spinning in different directions, this fourth quantum number is called the spin (s) quantum number. By convention, the allowed values of the spin quantum number are $+\frac{1}{2}$ and $-\frac{1}{2}$.

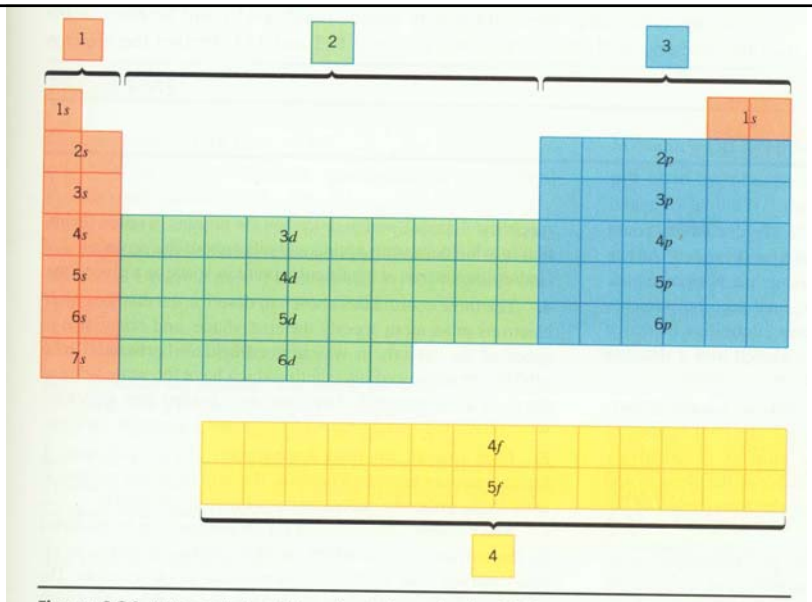
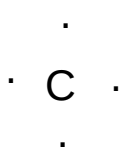


Figure 6.24 The periodic table reflects the order in which atomic orbitals are filled. The s orbitals are filled in the two columns on the far left and the p orbitals are filled in the six columns on the right. The d orbitals are filled along the transition between the s and p orbitals. The f orbitals are filled in the two long rows of elements at the bottom of the table.

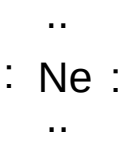
Outer shell or valence shell

Lewis structure and Octet rule

C: 6 electrons, $1s^2 2s^2 2p^2$

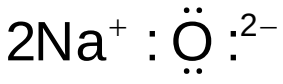


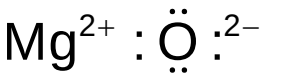
Ne: 10 electrons, $1s^2 2s^2 2p^6$



Chemical Bonding

- Ionic bond: is the electrostatic force of attraction between ions that carry opposite electrical charges.





- Covalent bond: is the force of attraction of one or more pairs of electrons that are shared between the bonded atoms.