# Inorganic pharmaceutical chemistry

## Lecture title

-Atomic and molecular structure/ Complexation.

-Essential and trace ions: Iron, copper, sulfur, iodine.

-Non essential ions: Fluoride, bromide, lithium, gold, silver and mercury.

-Gastrointestinal agents: Acidifying agents. Antacids.

-Protective adsorbents.

-Topical agents.

-Dental agents.

-Radiopharmaceutical preparations.

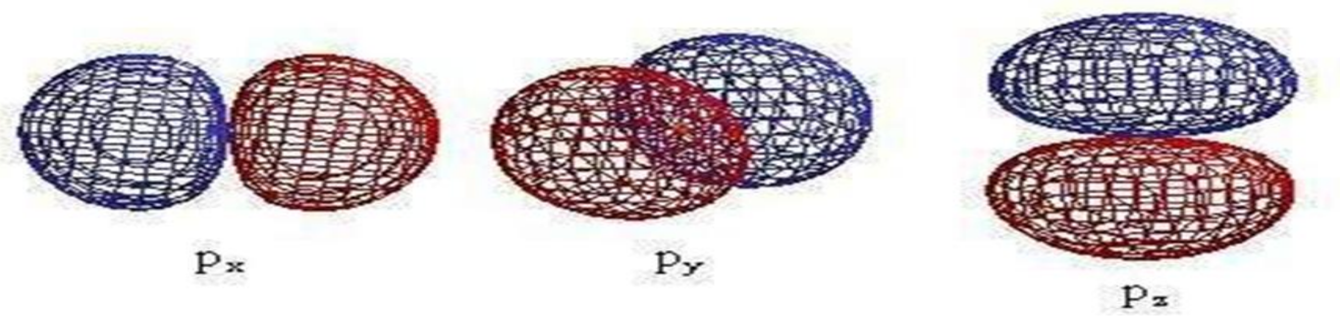
-Radio opaque and contrast media

# Atomic Orbitals

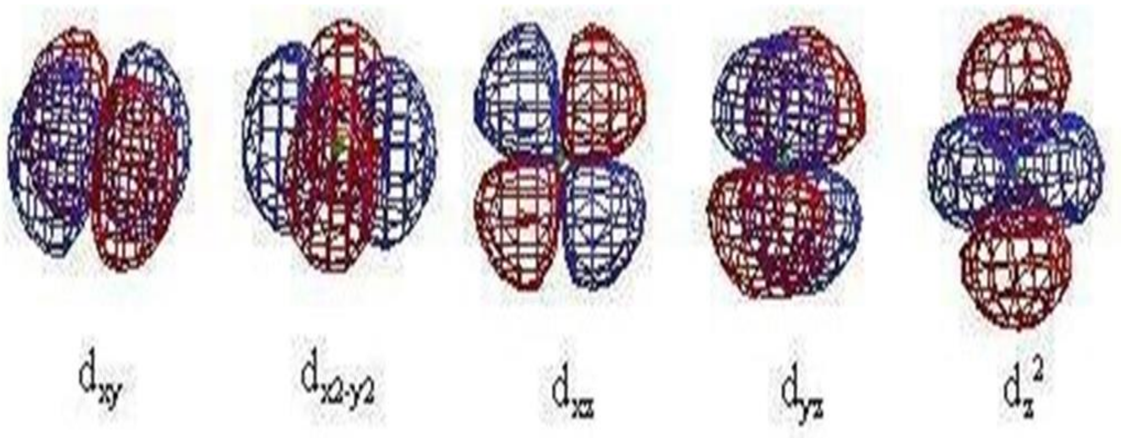
- **Heisenberg Principle**
- \- states that it is impossible to define what time and where an electron is and where is it going next. This makes it impossible to know exactly where an electron is traveling in an atom. Since it is impossible to know where an electron is at a certain time, a series of calculations are used to approximate the volume and time in which the electron can be located. These regions are called Atomic Orbitals. These are also known as the **quantum states of the electrons**

- Only two electrons can occupy one orbital and they must have different spin states, ½ spin and – ½ spin (easily visualized as opposite spin states).
- - Orbitals are grouped into subshells. And this field of study is called quantum mechanics atomic Subshells These are some examples of atomic orbitals:
- **S subshell**: (Spherical shape) There is one S orbital in an S subshell. The electrons can be located anywhere within the sphere centered at the atom's nucleus

- **P Orbitals**: (Shaped like two balloons tied together) There are 3 orbitals in a p subshell that are denoted as px, py, and pz orbitals. These are higher in energy than the corresponding S orbitals.



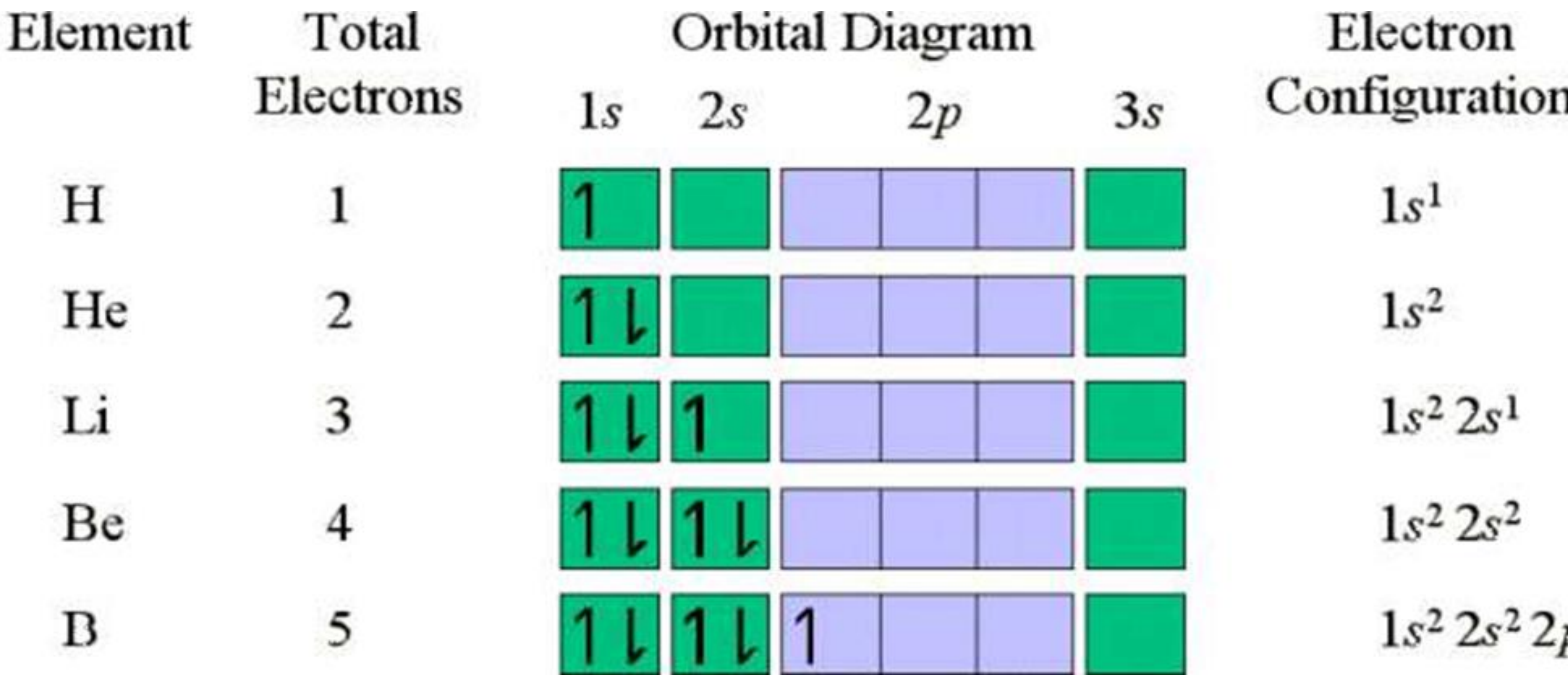
- **D Orbitals**: The d subshell is divided into 5 orbitals (dxy, dxz, dyz, dz 2 and dx 2 -y 2 ). These orbitals have a very complex shape and are higher in energy than the S and P orbitals



# Electronic configuration

- Every element is different.
- The number of protons determines the identity of the element.
- The number of electrons determines the charge.
- The number of neutrons determines the isotope.

- All chemistry is done at the electronic level (that is why electrons are very important).
- Electronic configuration is the arrangement of electrons in an atom. These electrons fill the atomic orbitals
    - Atomic orbitals are arrange by energy level (n) , subshells(l), orbital (ml) and spin (ms).



| Element | Total Electrons | Orbital Diagram 1s | 2s | 2p | | | 3s | Electron Configuration |
|---|---|---|---|---|---|---|---|---|
| H | 1 | ↑ | | | | | | $1s^1$ |
| He | 2 | ↑↓ | | | | | | $1s^2$ |
| Li | 3 | ↑↓ | ↑ | | | | | $1s^2 2s^1$ |
| Be | 4 | ↑↓ | ↑↓ | | | | | $1s^2 2s^2$ |
| B | 5 | ↑↓ | ↑↓ | ↑ | | | | $1s^2 2s^2 2p^1$ |

The two electrons in Helium represent the complete filling ofthe first electronic shell. Thus, the electrons in He are in a very stable configuration .
For Boron (5 electrons) the 5th electron must be placed in a 2*p* orbital because the 2*s* orbital is filled. Because the 2*p* orbitals are equal energy, it doesn't matter which 2*p* orbital isfilled

- Electronic configurations can also be written in a short hand which references the last completed orbital shell (i.e. all orbitals with the same principle quantum number'n' have been filled)

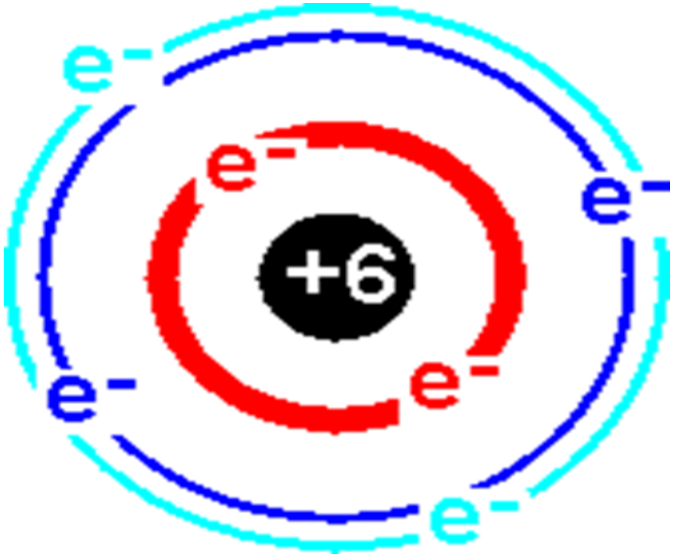
- The electronic configuration of Na(11) can be written as3s1
- The electronic configuration of  Li (3) can be written as2s1

- The electrons in the stable (Noble gas) configuration are

termed the core electrons
- The electrons in the outer shell (beyond the stable core)are called the valence electrons

# Valence Electrons

**The valence electrons are the electrons in the lastshell or energy level of an atom.**




Carbon - $1s^2 2s^2 2p^2$ -four valence electron

# *Examples of Electronic Configuration*

$Ne \rightarrow 1s^2\ 2s^2\ 2p^6$ (10 electrons)

$F \rightarrow 1s^2\ 2s^2\ 2p^5$ (9 electrons)

$F^- \rightarrow 1s^2\ 2s^2\ 2p^6$ (10 electrons)

$Mg \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s^2$ (12 electrons)

$Mg^{2+} \rightarrow 1s^2\ 2s^2\ 2p^6$ (10 electrons)

# The Quantum Mechanical Model

- A quantum is the amount of energy needed to move from one energy level to another.
- Since the energy of an atom is never "in between" there must be a quantum leap in Energy.

# Quantum Numbers

Each orbital describes a spatial distribution of electron density. An orbital is described by a set of three quantum numbers.

# Principal Quantum Number, *n*

- The principal quantum number, *n*, describes the energylevel on which the orbital resides.
- The values of *n* are integers $\geq 0$.
- This quantum number defines the shape of the orbital.
- Allowed values of *l(Subshell)* are integers ranging from 0to $n - 1$.We use letter designations to communicate the different values of *l* and, therefore, the shapes andtypes of orbitals.

| Value of l | 0 | 1 | 2 | 3 |
|---|---|---|---|---|
| Type of orbital | *s* | *p* | *d* | *f* |

# Magnetic Quantum Number, $m_l$

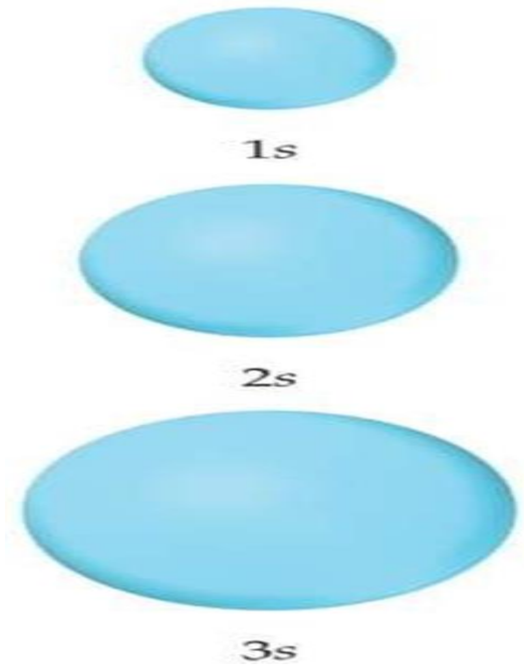
Describes the three-dimensional orientation of the orbital.

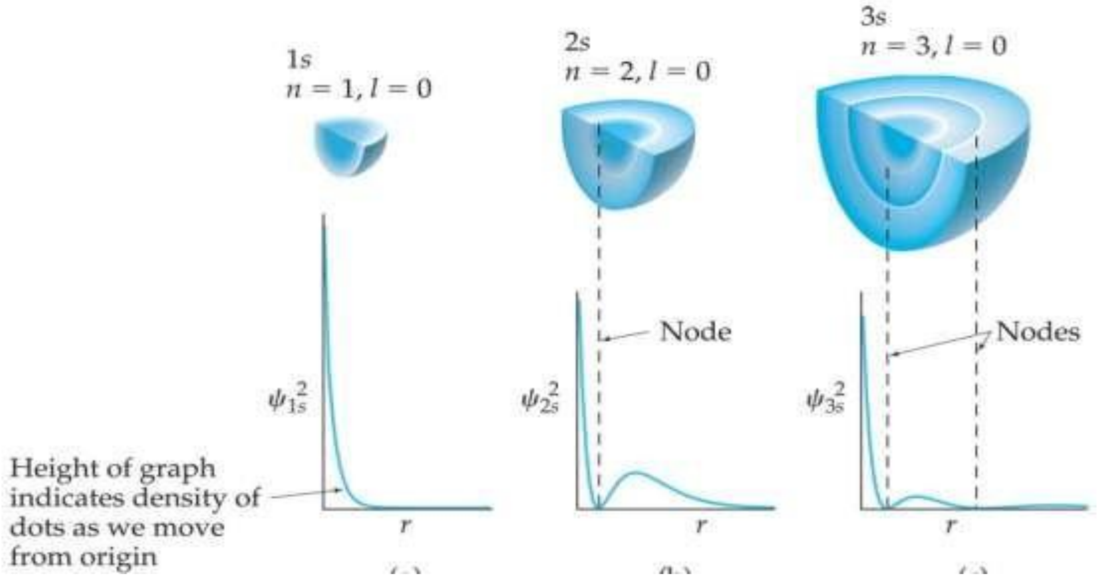
- Values are integers ranging from $-l$ to $l$: $-l \leq m_l \leq l$.
- Therefore, on any given energy level, there can be up to 1 *s* orbital, 3 *p* orbitals, 5 *d* orbitals, 7 *f* orbitals, etc.
- Orbitals with the same value of *n* form a shell.
- Different orbital types within a shell are subshells.

| $n$ | Possible Values of $l$ | Subshell Designation | Possible Values of $m_l$ | Number of Orbitals in Subshell | Total Number of Orbitals in Shell |
|---|---|---|---|---|---|
| 1 | 0 | 1*s* | 0 | 1 | 1 |
| 2 | 0 | 2*s* | 0 | 1 | |
| | 1 | 2*p* | 1, 0, −1 | 3 | 4 |
| 3 | 0 | 3*s* | 0 | 1 | |
| | 1 | 3*p* | 1, 0, −1 | 3 | |
| | 2 | 3*d* | 2, 1, 0, −1, −2 | 5 | 9 |
| 4 | 0 | 4*s* | 0 | 1 | |
| | 1 | 4*p* | 1, 0, −1 | 3 | |
| | 2 | 4*d* | 2, 1, 0, −1, −2 | 5 | |
| | 3 | 4*f* | 3, 2, 1, 0, −1, −2, −3 | 7 | 16 |

# *s* Orbitals

- Value of $l = 0$.
- Spherical in shape.
- Radius of sphere increases with increasing value of *n*.

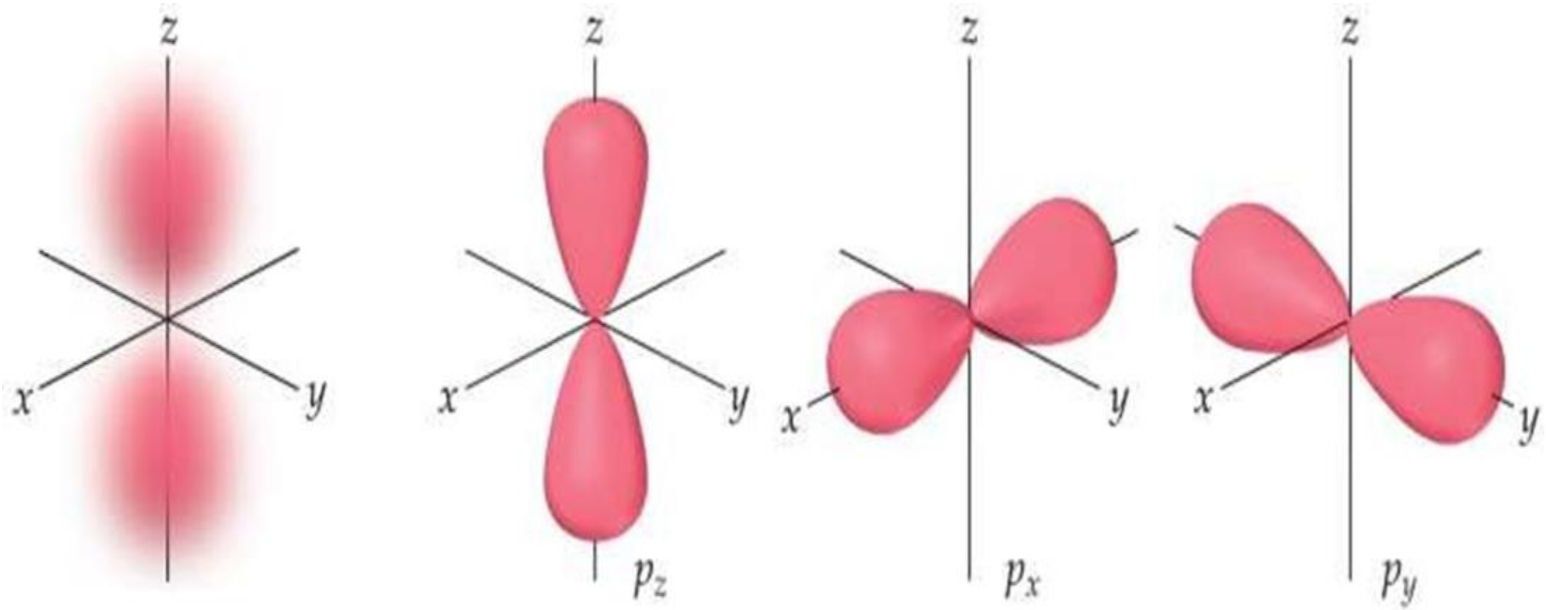




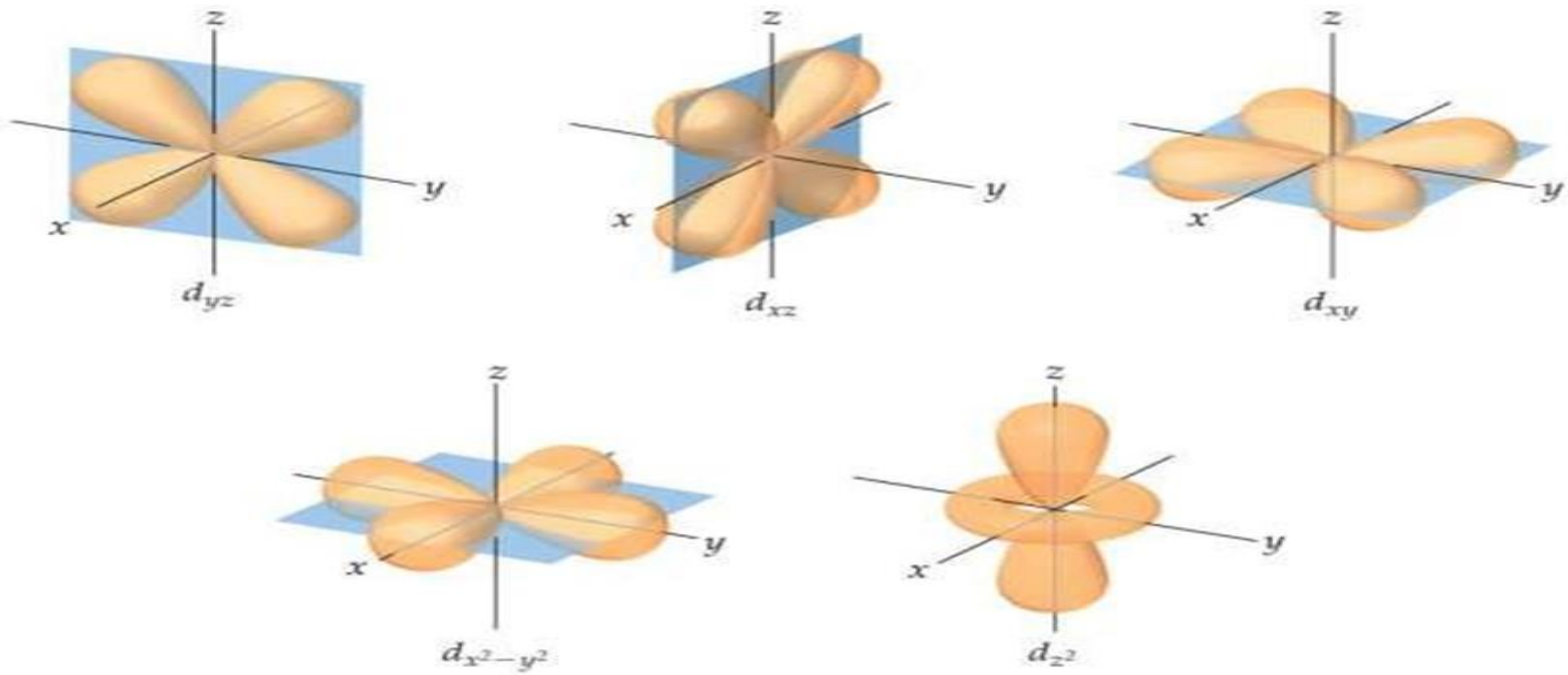

Observing a graph of probabilities of finding an electron versus distance from the nucleus, we see that *s* orbitals possess $n$–1 nodes, or regions where there is 0 probability of finding an electron.

# *p* Orbitals

- Value of $l$= 1
- Have two lobes with a node between them.



# *d* Orbitals

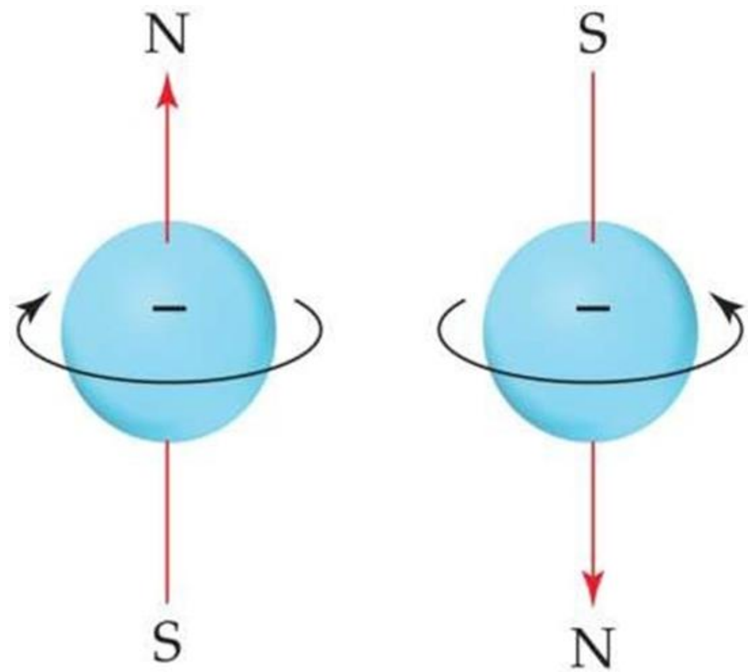



– Value of *l* is 2.

Four of the five orbitals have 4 lobes; the other resembles a *p* orbital with a doughnut around the center.

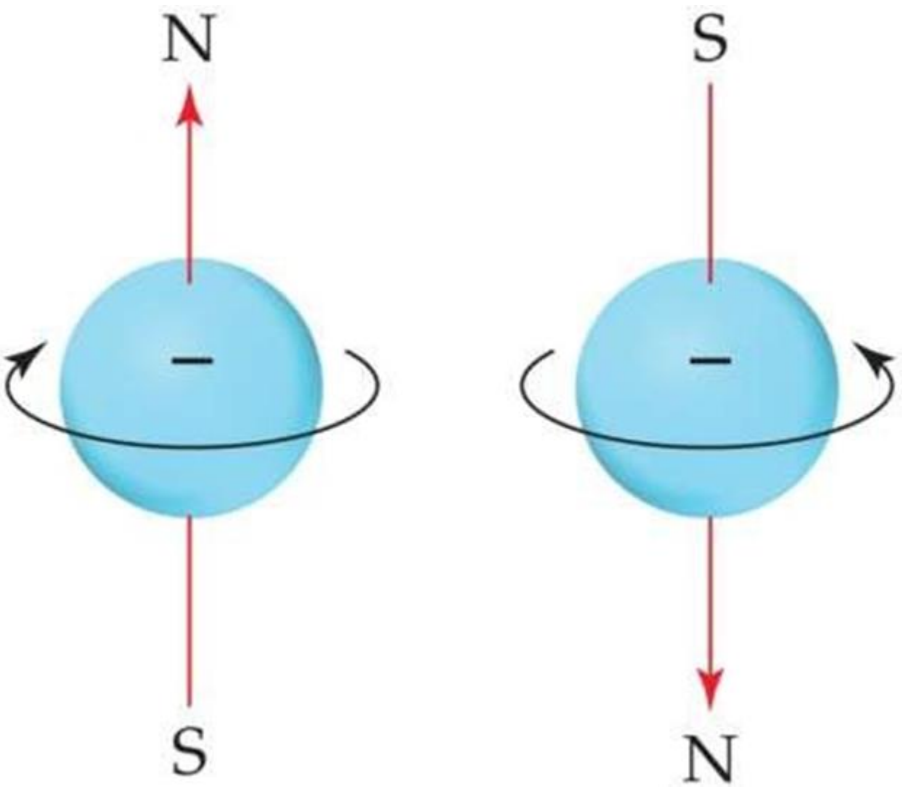
# Spin Quantum Number, $m_s$

- The two electrons in the sameorbital do not have exactly the same energy.
- The “spin” of an electron describes its magnetic field, whichaffects its energy.
- This led to a fourth quantumnumber, the spin quantum number, $m_s$.
- The spin quantum number has only 2 allowed values: +1/2 and −1/2.



# Pauli Exclusion Principle

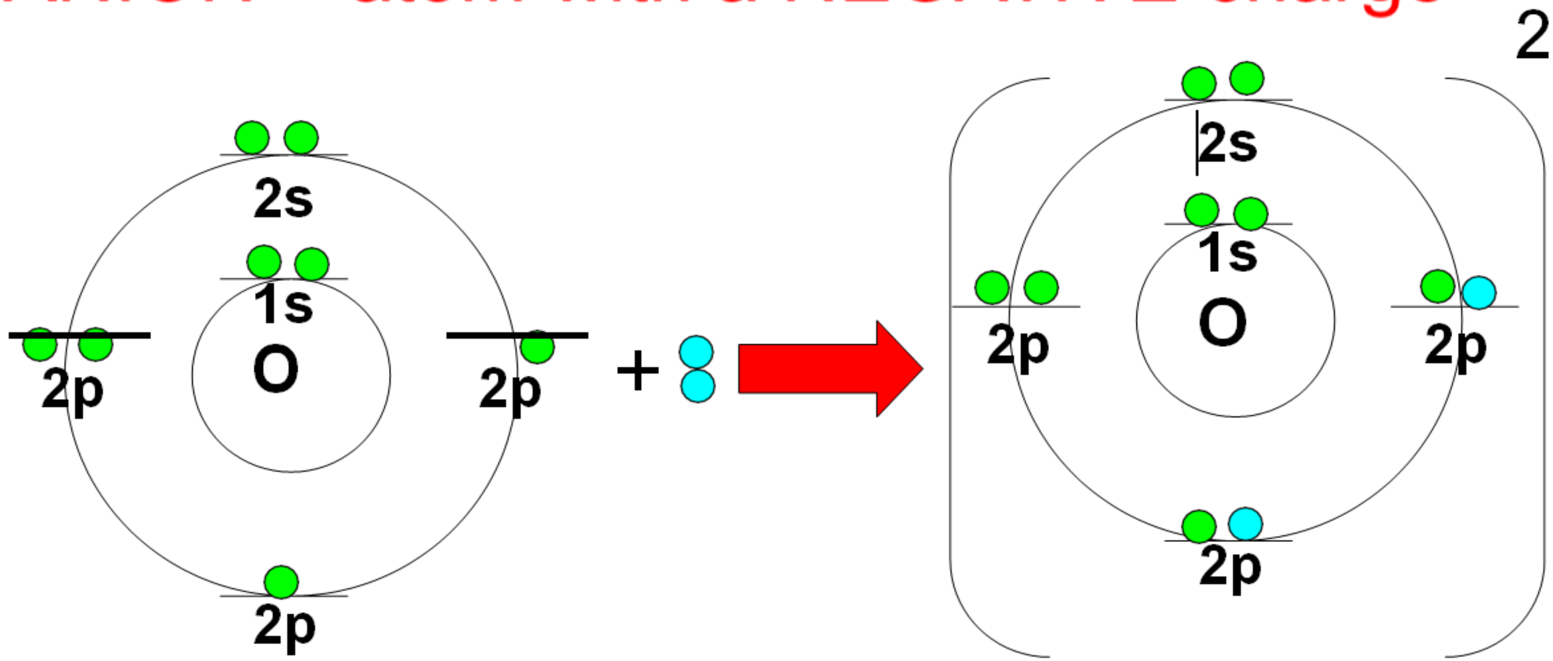
- No two electrons in the same atom can have exactly the same energy.
- For example, no two electrons in the same atom can have identical sets of quantum numbers.



# Ionization

- When an atom gains an electron, it becomes negatively charged (more electrons than protons ) and is called an **anion.**
  - In the same way that nonmetal atoms can gain electrons
  - metal atoms can lose electrons and they become
    - positively charged **cations**.
  - Cations are always smaller than the original atom.
- Conversely, anions are always larger than the original atom

# ANION = atom with a NEGATIVE charge

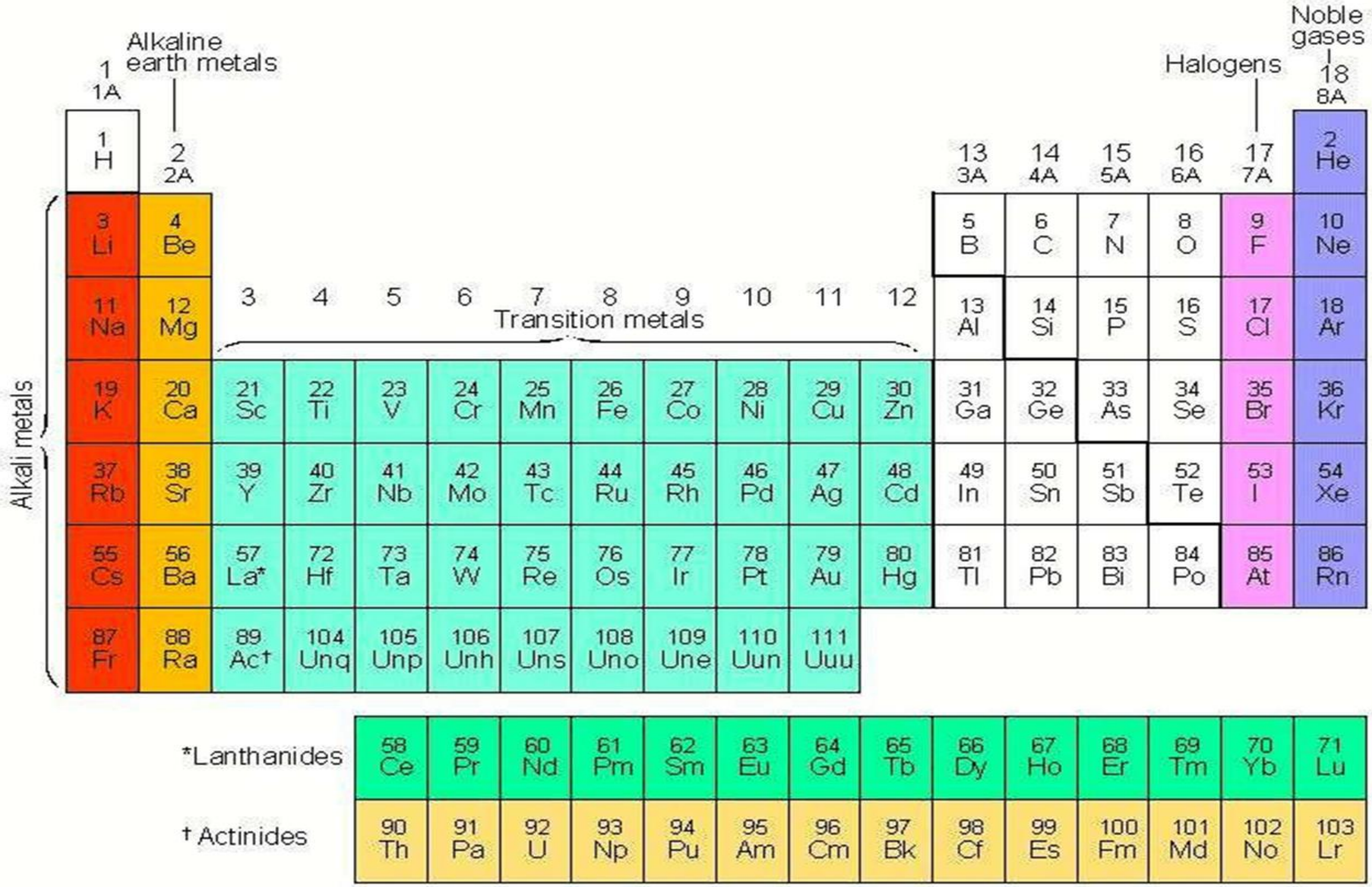



$$O + 2e^- \rightarrow O^{2-}$$

- Oxidation states:- The elements of boron family have $2s^2 2p^1$ configuration which means that they have 3 valance electron available for bond formation. By loosing these electrons they are accepted to show +3 oxidation states in there compounds.

- ***The Periodic Law***
-
  - When elements are arranged in order of increasing atomic number, there is a periodic repetition of their physical and chemical properties.
  - Horizontal rows = periodsThere are 7 periods
  - Vertical column = group (or family)Similar physical chemical prop.

    Identified by number & letter (IA, IIA)



Alkaline earth metals
Noble gases
Halogens
Alkali metals
Transition metals
1 1A
2 2A
3
4
5
6
7
8
9
10
11
12
13 3A
14 4A
15 5A
16 6A
17 7A
18 8A
1 H
2 He
3 Li
4 Be
5 B
6 C
7 N
8 O
9 F
10 Ne
11 Na
12 Mg
13 Al
14 Si
15 P
16 S
17 Cl
18 Ar
19 K
20 Ca
21 Sc
22 Ti
23 V
24 Cr
25 Mn
26 Fe
27 Co
28 Ni
29 Cu
30 Zn
31 Ga
32 Ge
33 As
34 Se
35 Br
36 Kr
37 Rb
38 Sr
39 Y
40 Zr
41 Nb
42 Mo
43 Tc
44 Ru
45 Rh
46 Pd
47 Ag
48 Cd
49 In
50 Sn
51 Sb
52 Te
53 I
54 Xe
55 Cs
56 Ba
57 La*
72 Hf
73 Ta
74 W
75 Re
76 Os
77 Ir
78 Pt
79 Au
80 Hg
81 Tl
82 Pb
83 Bi
84 Po
85 At
86 Rn
87 Fr
88 Ra
89 Ac†
104 Unq
105 Unp
106 Unh
107 Uns
108 Uno
109 Une
110 Uun
111 Uuu
*Lanthanides
58 Ce
59 Pr
60 Nd
61 Pm
62 Sm
63 Eu
64 Gd
65 Tb
66 Dy
67 Ho
68 Er
69 Tm
70 Yb
71 Lu
† Actinides
90 Th
91 Pa
92 U
93 Np
94 Pu
95 Am
96 Cm
97 Bk
98 Cf
99 Es
100 Fm
101 Md
102 No
103 Lr

# *Areas of the periodic table*

Three classes of elements are:

1) metals, 2) nonmetals, and Metalloids

1. Metals: electrical conductors, have luster, ductile,malleable
2. Nonmetals: generally brittle and non-lustrous, poor conductors of heat and electricity

    Some nonmetals are gases (O, N, Cl); some are brittle solids(S); one is a fuming dark red liquid (Br)

Notice the heavy, stair-step line?

1. Metalloids: border the line-2 sides .Properties are intermediate between metals andnonmetals

# Classifying the Elements

Classify elements based on electron configuration