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 and Molecular Structure /complexation

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Lecture 1

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.

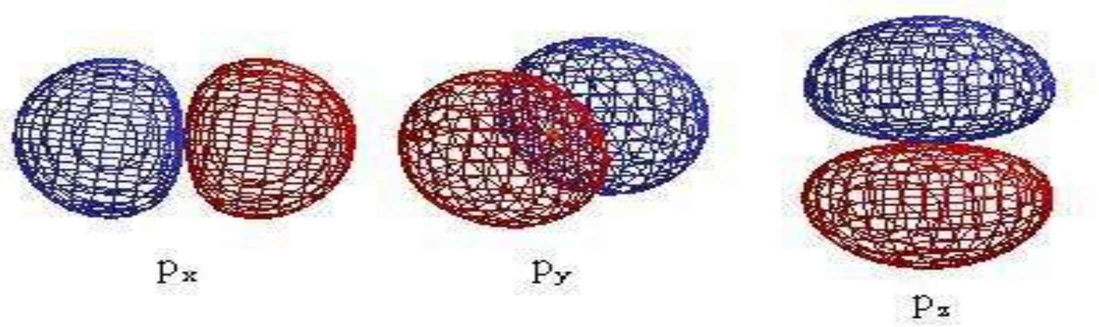
And this field of study is called quantum mechanics

Atomic Subshells

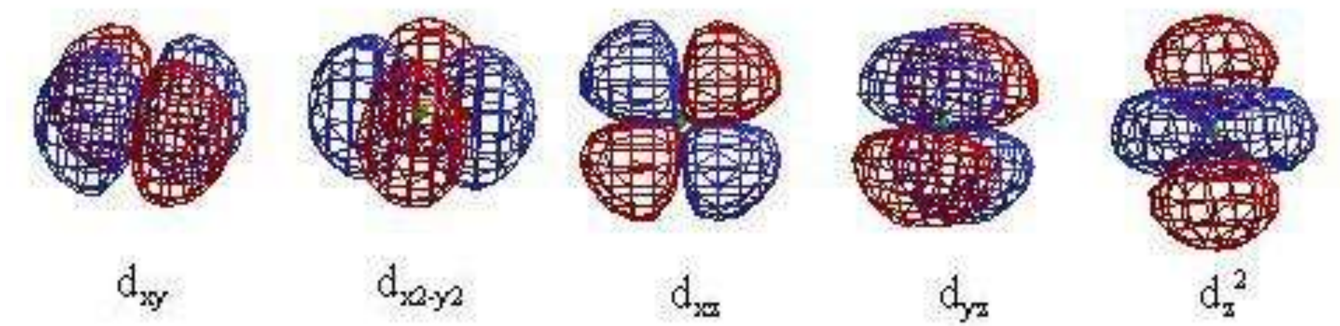
These are some examples of atomic orbitals:

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 (d_{xy}, d_{xz}, d_{yz}, d_{z^2} and $d_{x^2-y^2}$). 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 of the 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 is filled

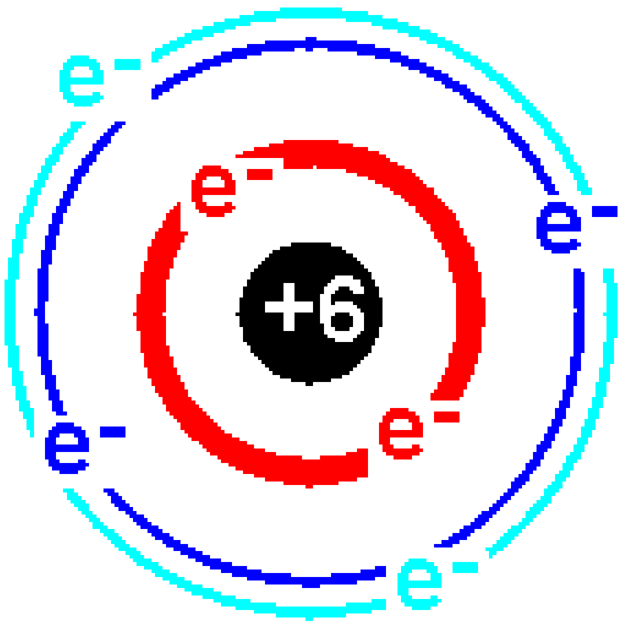
Electronic configurations can also be written in a short hand which references the last completed orbital shell (i.e. all orbitals with the same principle quantum number 'n' have been filled)

The electronic configuration of Na(11) can be written as 3s1
The electronic configuration of Li (3) can be written as 2s1

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 last shell or energy level of an atom.



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

Examples of Electronic Configuration

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

F → $1s^2\ 2s^2\ 2p^5$ (9 electrons)

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

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

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

Notice – different elements can have the same number of 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 energy level on which the orbital resides.
- The values of *n* are integers ≥ 0.
- This quantum number defines the shape of the orbital.
- Allowed values of *l(Subshell)* are integers ranging from 0 to *n* − 1.
- We use letter designations to communicate the different values of *l* and, therefore, the shapes and types of orbitals.

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

Magnetic Quantum Number, m_l

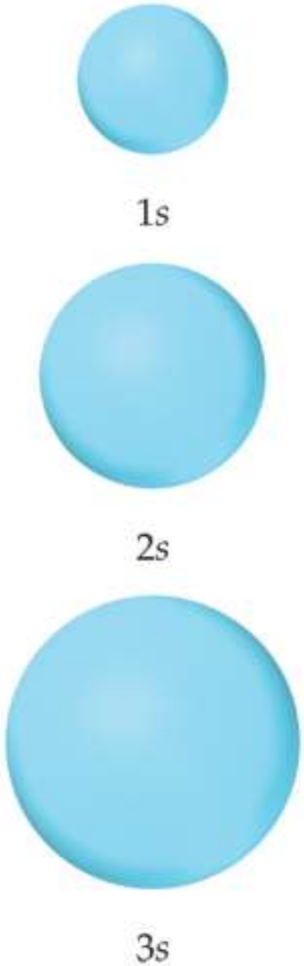
- Describes the three-dimensional orientation of the orbital.
- Values are integers ranging from -*l* to *l*: $-l \leq m_l \leq l$.
- Therefore, on any given energy level, there can be up to 1 *s* orbital, 3 *p* orbitals, 5 *d* orbitals, 7 *f* orbitals, etc.
- Orbitals with the same value of *n* form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

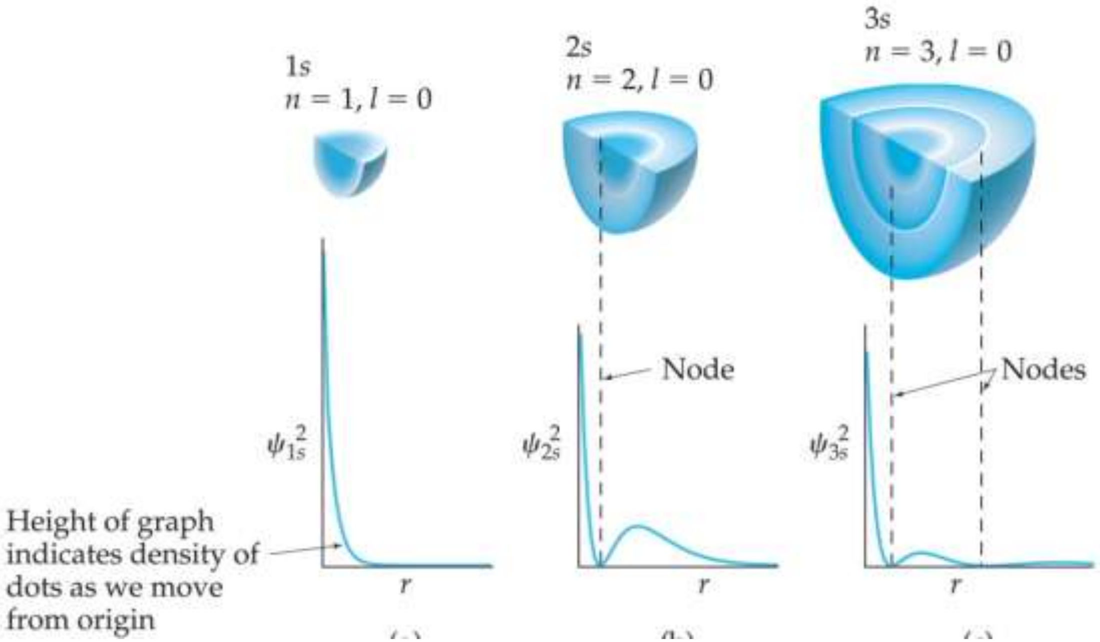
Allowed Sets of Quantum Numbers for Electrons in Atoms

Level n	**1**	**2**				**3**								
Sublevel ℓ	0	0	1			0	1			2				
Orbital $\mathbf{m}_{\ell}$	0	0	1	0	-1	0	1	0	-1	2	1	0	-1	-2
Spin $\mathbf{m}_s$ ↑ = +1/2 ↓ = -1/2	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓

s Orbitals



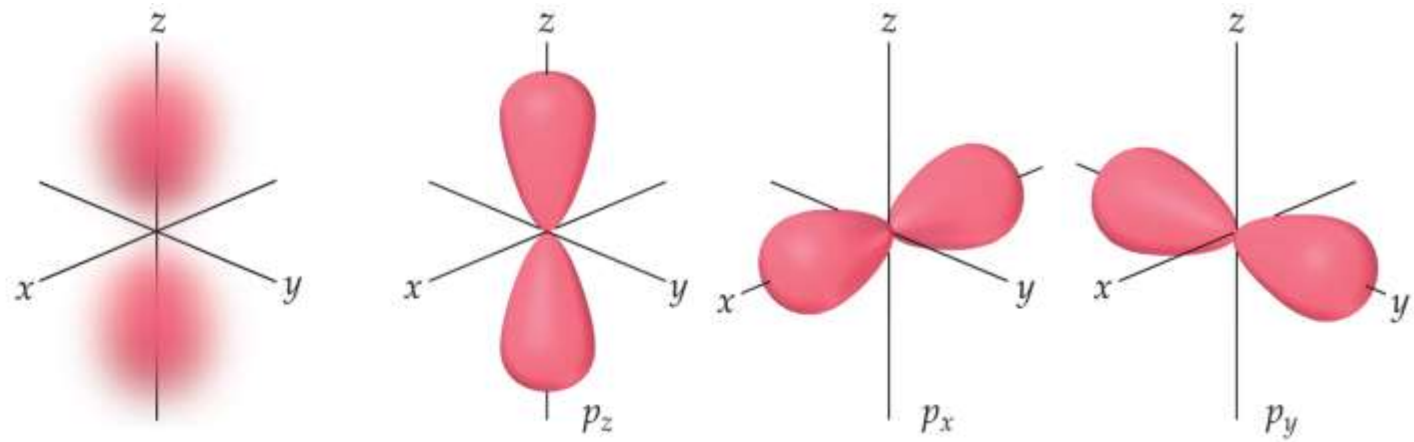
- Value of *l* = 0.
- Spherical in shape.
- Radius of sphere increases with increasing value of *n*.



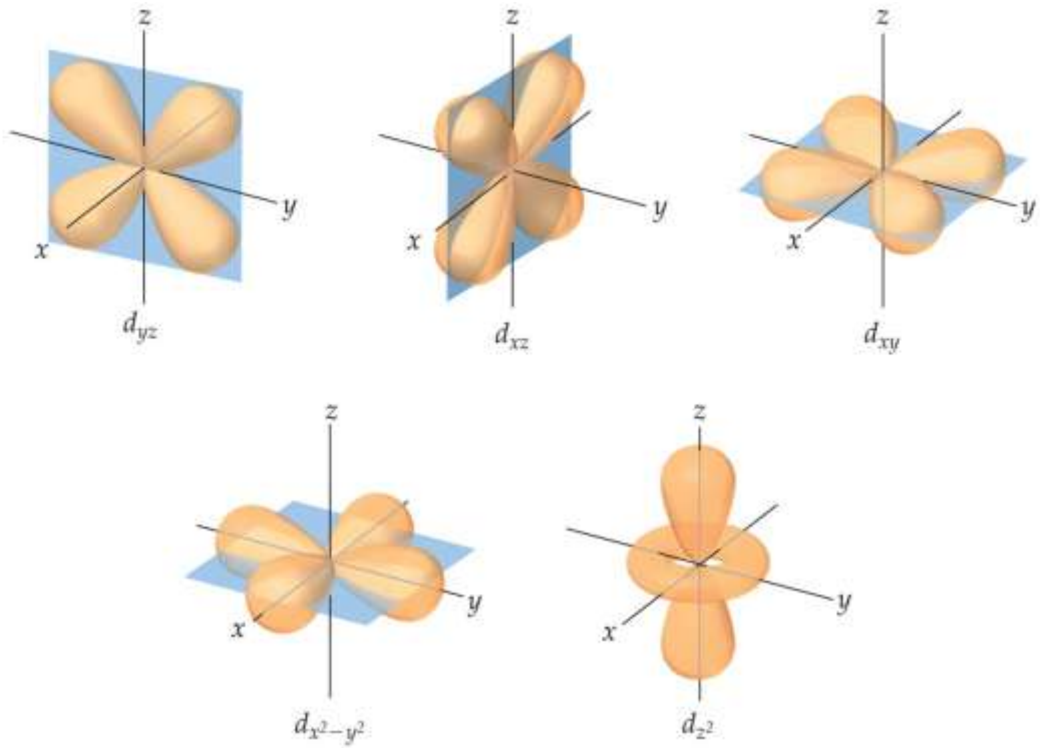
Observing a graph of probabilities of finding an electron versus distance from the nucleus, we see that *s* orbitals possess *n*−1 nodes, or regions where there is 0 probability of finding an electron.

p Orbitals

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



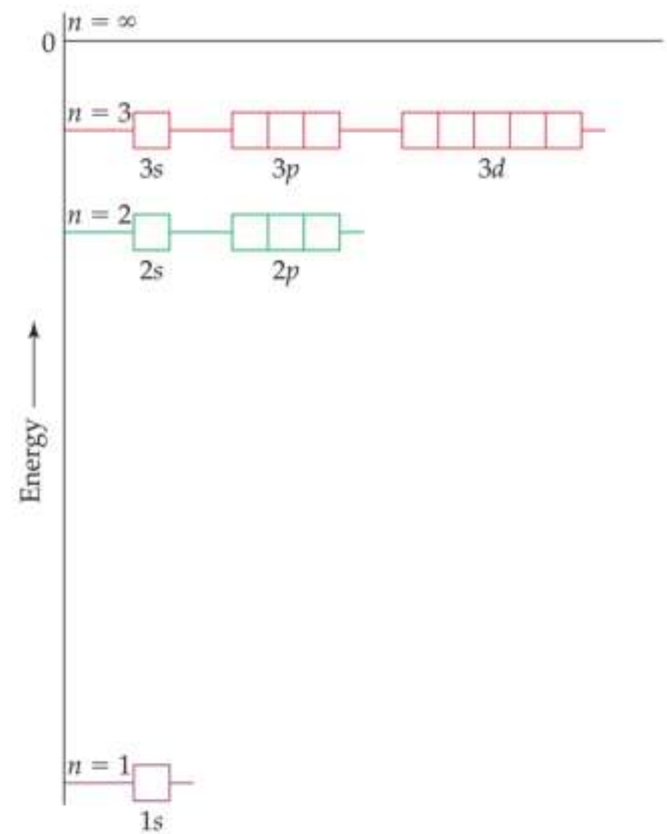
d Orbitals

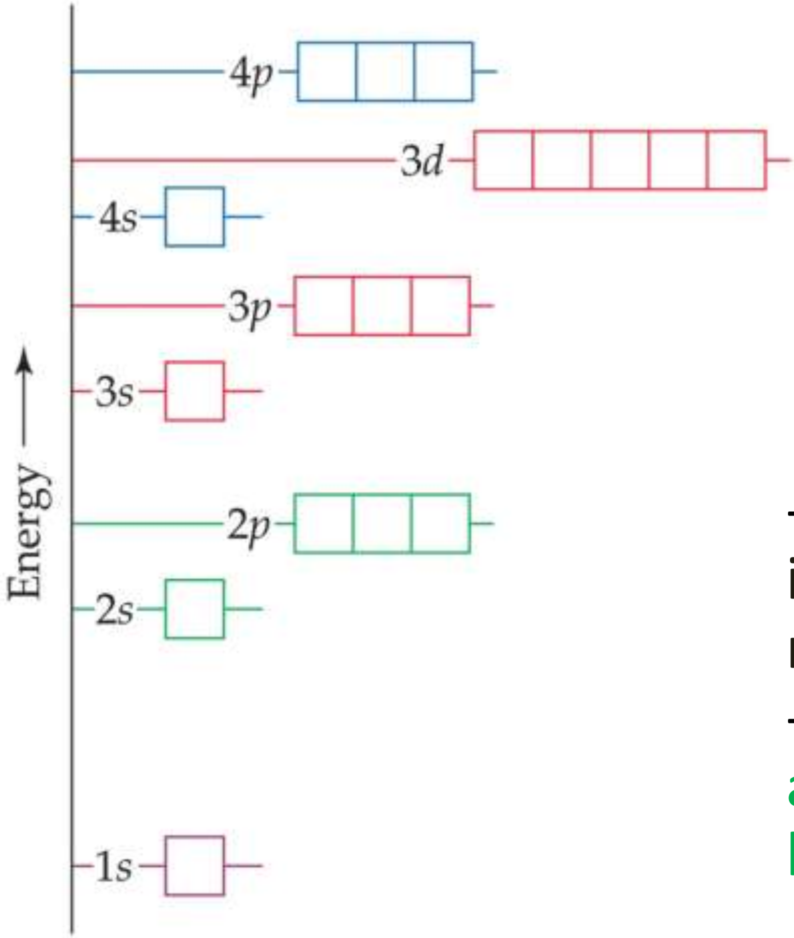


- Value of *l* is 2.
- Four of the five orbitals have 4 lobes; the other resembles a *p* orbital with a doughnut around the center.

Energies of Orbitals

- For a one-electron hydrogen atom, orbitals on the same energy level have the - same energy. That is, they are degenerate.

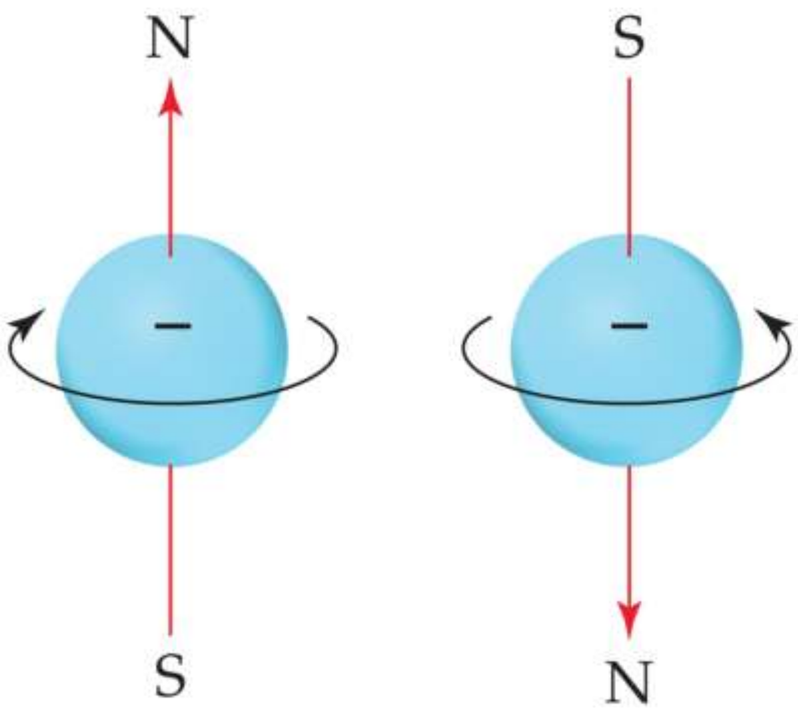




- As the number of electrons increases, though, so does the repulsion between them.
- Therefore, in many-electron atoms, orbitals on the same energy level are no longer degenerate.

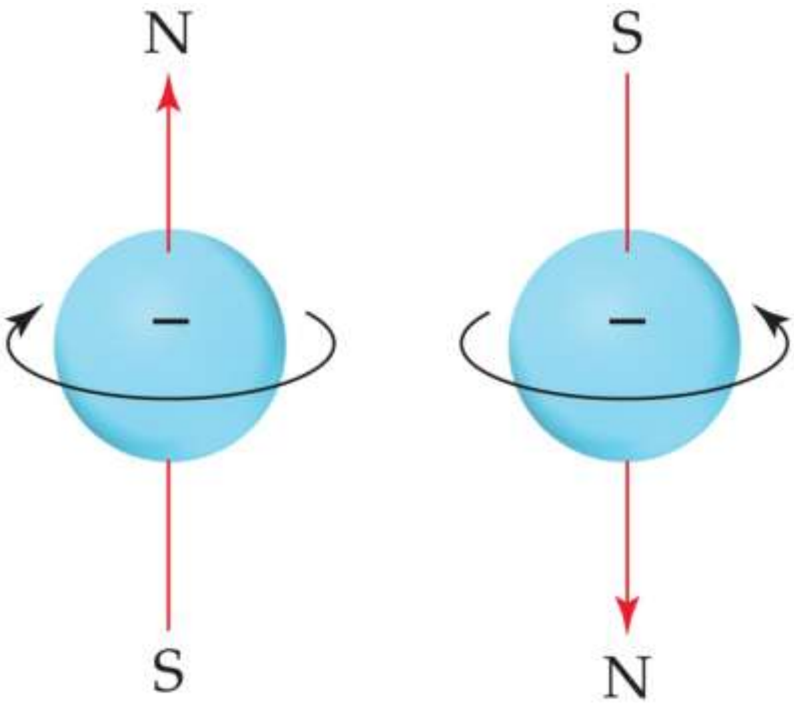
Spin Quantum Number, m_s

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



Pauli Exclusion Principle

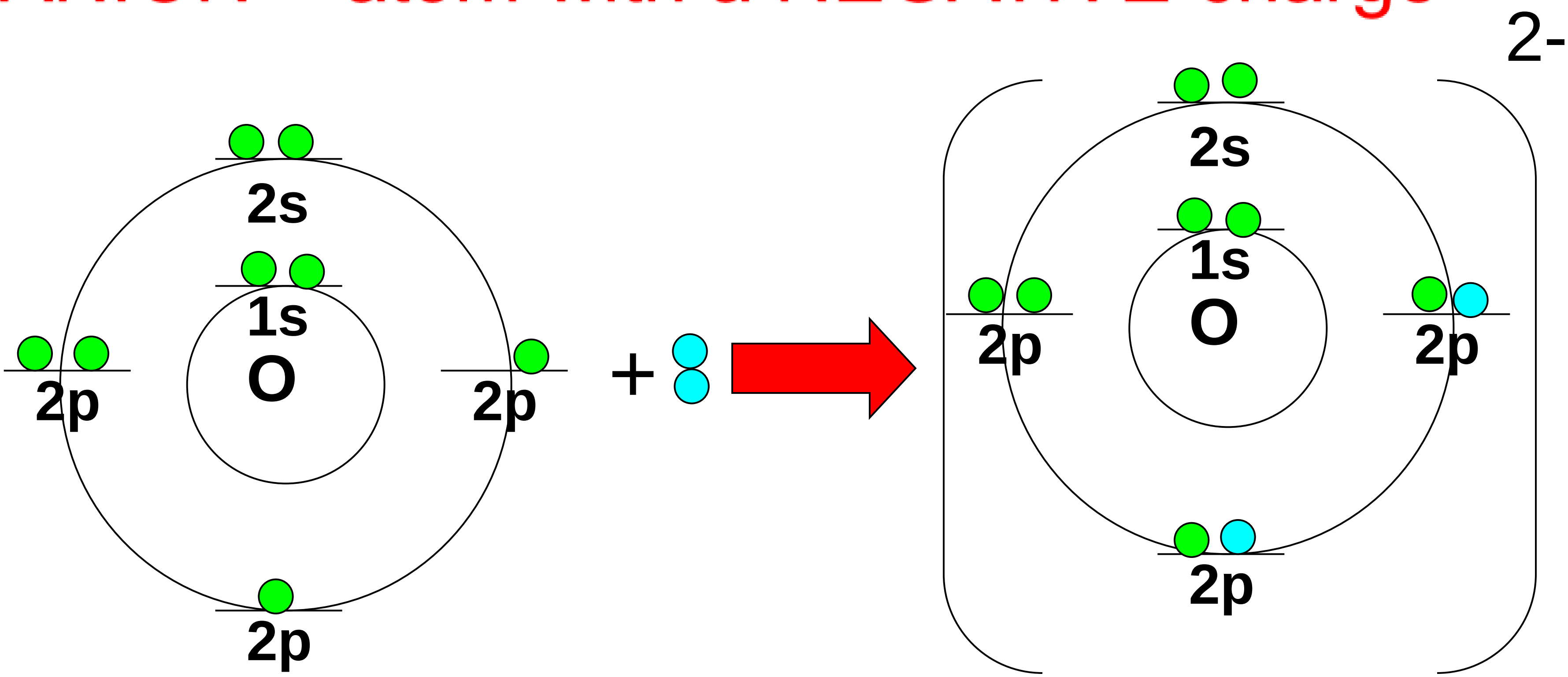
- No two electrons in the same atom can have exactly the same energy.
- For example, no two electrons in the same atom can have identical sets of quantum numbers.



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.

- Valance electrons for transition elements reside in the ns and (n-1) d subshells.

Table 22.1 Electron Configurations of the Fourth-Period Transition Elements

	spdf Configu-ration	Box Notation 3*d*					4*s*
Sc	$[Ar]3d^14s^2$	↑					↑↓
Ti	$[Ar]3d^24s^2$	↑	↑				↑↓
V	$[Ar]3d^34s^2$	↑	↑	↑			↑↓
Cr	$[Ar]3d^54s^1$	↑	↑	↑	↑	↑	↑
Mn	$[Ar]3d^54s^2$	↑	↑	↑	↑	↑	↑↓
Fe	$[Ar]3d^64s^2$	↑↓	↑	↑	↑	↑	↑↓
Co	$[Ar]3d^74s^2$	↑↓	↑↓	↑	↑	↑	↑↓
Ni	$[Ar]3d^84s^2$	↑↓	↑↓	↑↓	↑	↑	↑↓
Cu	$[Ar]3d^{10}4s^1$	↑↓	↑↓	↑↓	↑↓	↑↓	↑
Zn	$[Ar]3d^{10}4s^2$	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓

Metal reactions

- All metals undergo oxidation with oxygen, halogens, aqueous acids.
- First the outer most electron is removed, followed by one or more d electrons.
- Some generate cations with unpaired electrons = Para magnetism.
- Are colored.
- For first transition series common oxidation numbers are +2 and +3.

Fe: $3d^6 4s^2$

$Fe + O_2 \longrightarrow Fe_2O_3$
Fe^{3+}
$3d^5$

$Fe + Cl_2 \longrightarrow FeCl_3$
Fe^{3+}
$3d^5$

$Fe + HCl \longrightarrow FeCl_2 + H_2$
Fe^{2+}
$3d^6$

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 = periods

There are 7 periods

- Vertical column = group (or family)

Similar physical & chemical prop.

Identified by number & letter (IA, IIA)

Alkaline earth metals (group 2)

Halogens (group 17)

Noble gases (group 18)

Transition metals (groups 3–12)

Alkali metals (group 1)

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 3) 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?

3-Metalloids: border the line-2 sides

Properties are intermediate between metals and nonmetals

Classifying the Elements

<u>Classify</u> elements based on electron configuration