بسم الله الرحمن الرحيم

مرحبا بكم في بداية العام الدراسي الجديد

٢٠١٤ـ٢٠١٥

University of karbala
Collage of pharmacy
3rd Stage

- Course title :
- Inorganic medicinal and Pharmaceutical Chemistry

Theory: 2hour **Lab**: 3hr

- **Course content**: Inorganic medicinal and Pharmaceutical Chemistry has been designed for two purposes:

First

- 1-To present a review of those principle of inorganic chemistry that apply to medicinal and Pharmaceutical Chemistry. The first two chapters are devoted to explanation of atomic structure as it relates to bonding forces and complexation , and summary of important physical properties of each element group from the periodic table .

Second

- 2-The second purpose is to present details discussions of these inorganic reagents used as pharmaceutical aids and necessities or therapeutic (علاجي) and diagnostic(التشخيصي) agents.

Reference Book:

- Inorganic medicinal and Pharmaceutical Chemistry by Block.Roche .Soine.Wilson .1986
- Inorganic medicinal and Pharmaceutical Chemistry by JN Delgado and w.A.Remers 1998.

Lec.:One Date: 3 / 10/2010

- **Lec Title : Electronic structure of atoms:**
- **Part (One)(1-5)**

- **The fundamental unit of any matter is the atom.**
- **The various chemical and physical properties of any matter are determined by its chemical composition.**

- **Element** are composed of like atoms and isotopes. Example Bromine Br .
- **Isotopes:** they are different in the neutrons number so they are different in the atomic mass

Sub atomic particles:

- Atoms are composed of a central nucleus surrounds by electrons which occupied different region of space.
- The nucleus is composed of two types of stable particles which comprised most of the mass of the atom.
- These particles are protons and neutrons which are held together by nuclear forces.

Neutron & Proton

- **Neutron** : its uncharged particle with amass of 1.675x10-24 gm or 1.009 **a.m.u**(atomic mass unit)
- **Proton**: its positively charged particle with mass slightly less than that of neutrons.

mass of proton

- mass of proton= 1.672×10^{-24}gm or 1.008 a.m.u
- Every stable atom has certain number of protons (equal number of electrons)
- This is in neutral atom and with a particle number of neutrons.
- The sum of masses of both neutrons and proton is the atomic mass.

- Mass of proton + mass of n=Atomic mass
- n.of protons =n.of electrons =Atomic number
- electron : it is negative charge particle has very small mass $9.107x10^{-28}$gm or 0.0006a.m.u.
- Mass of electron = 1/1840 of that of proton

TABLE 2.1 A Comparison of Subatomic Particles

	Mass		Charge	
Particle	grams	amu*	coulombs	e
Electron	$9.109\,382 \times 10^{-28}$	$5.485\,799 \times 10^{-4}$	$-1.602\,176 \times 10^{-19}$	-1
Proton	$1.672\,622 \times 10^{-24}$	$1.007\,276$	$+1.602\,176 \times 10^{-19}$	$+1$
Neutron	$1.674\,927 \times 10^{-24}$	$1.008\,665$	0	0

- **Unstable sub atomic particles;**
- These are observed when atoms are bonded by any type of particles.
- Among this unstable subatomic particle there are:
- positron: it’s the direct counter part of electron it has the same mass of electron but oppositely charged(+).

- **Betatron or negatron or beta particle (ß) it is an electron emitted from the nucleus .**
- **Neutrin: its also a part of neutron is uncharged species with zero mass are detected through the bombardment of nucleus.**

Atomic Orbital:

- **Laws of quantum mechanics :**
  - **The energy description of electrons was by Niels Bohr in 1913.**
  - **Bohr gave the planetary picture(الصورة الكوكبية) of atom.**

- **Electrons were considered as particles revolved or moved around the nucleus in stationary planer or orbitals and which have definite energies**

- ***Bohr model*** succeed in the description of hydrogen atom which contain one electron.
- But it could not succeed in atoms contain more than one electron.

- ***De Broglies*** work in 1924 developed the theory of quantum mechanics which related the velocity and momentum (الزخم) to the dual particle-wave nature of electron

- ***Schrödinger's*** development of an equation in 1926 which known as the wave equation.
- Electrons are present in desecrate volumes of space about nucleus

- The spaces are named atomic orbitals the electrons are contained within these orbitals described by asset of four quantum.
- The uncertainty principle of Heisenberg states that :
- It is not possible to fix simultaneously the momentum and the position of an electron. So its necessary to discuss the location of electron in atoms or molecules in terms of probability.

- **The first three quantum numbers refer to some property of the space or orbitals while the fourth one describes the spin of electron**

1-The principle quantum number (n):

- This number is given the symbol (n) and the quantum theory states that electrons in atoms exist in discrete energy levels. The energy associated with the electron increase as it locates for the form the nucleus. The principle quantum number describes:

The principle quantum number describes:

- 1-The relative positions of these energy levels.
- 2- Their distance from the nucleus.
- 3-possibility of discontinuities or points of zero probability in the levels

- **n: is integer number could be 1,2,3……α.**
- **When n=1 the electron is found in the energy level closet to nucleus.**
- **In the older literature the shells referred to as k,L,M…..etc correspond to n=1,2,3….etc**

The sub orbital quantum number (*l* l) **The angular-momentum quantum number**

- **(*l*)** this number given the symbol (*l*) .
  - **The volume of space which represents the region of greatest probability of finding an electron varies in shape and size, depending upon the energy level.**
  - **The sub orbital quantum number describes the shape of the orbital or the electron cloud.**

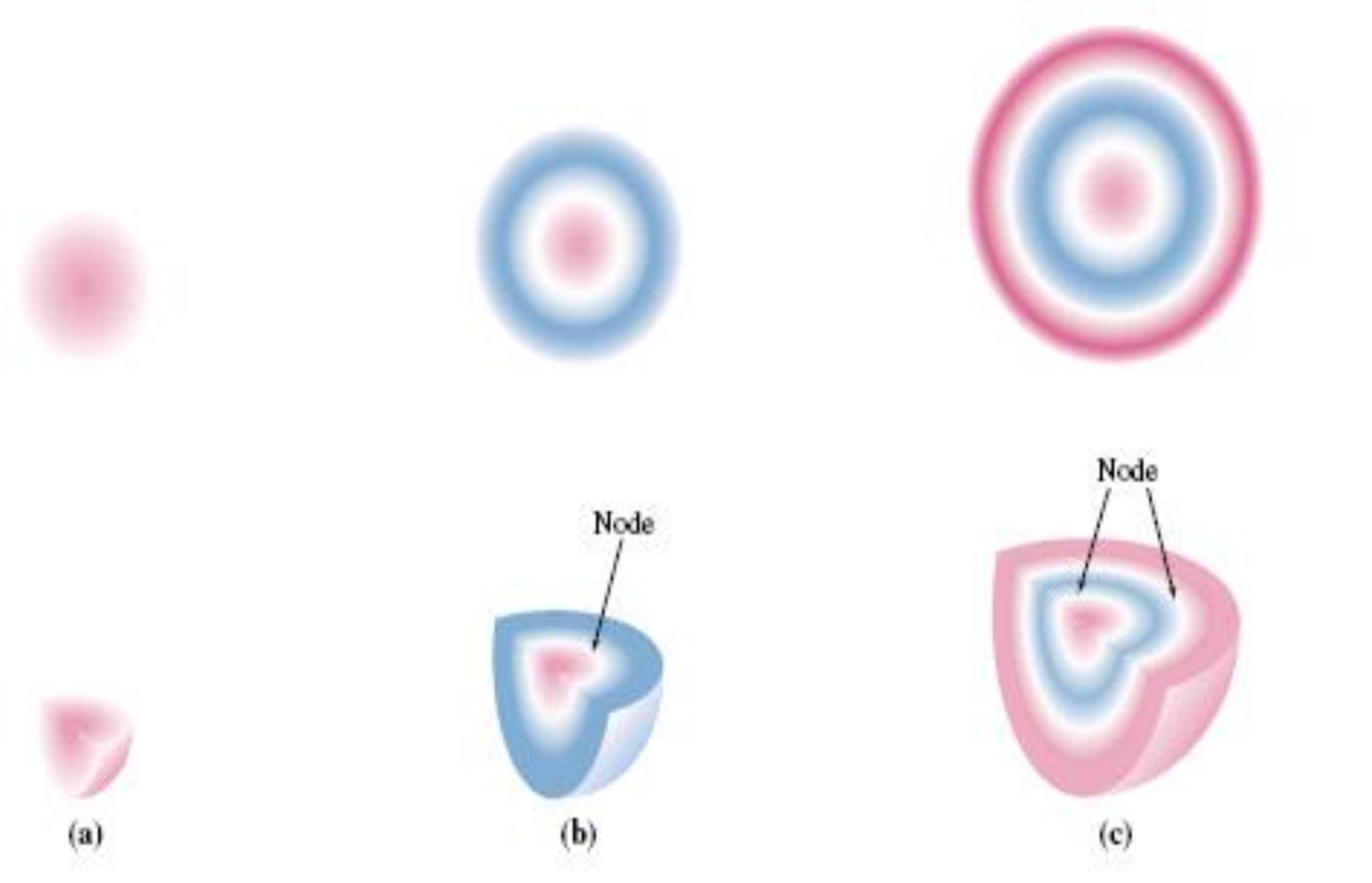
- ***l*)**:is integer number limited by the corresponding value of n .l =0,1,2,…..
- (n-1)
- Such as if n=1 → l = 0 .
- If n=2 → l= 0, 1

- A Second designation for the orbitals described by various values of(***l***) is in common use. The use of the letters s ,f .d and f for orbitals having the following sub orbital number is important .

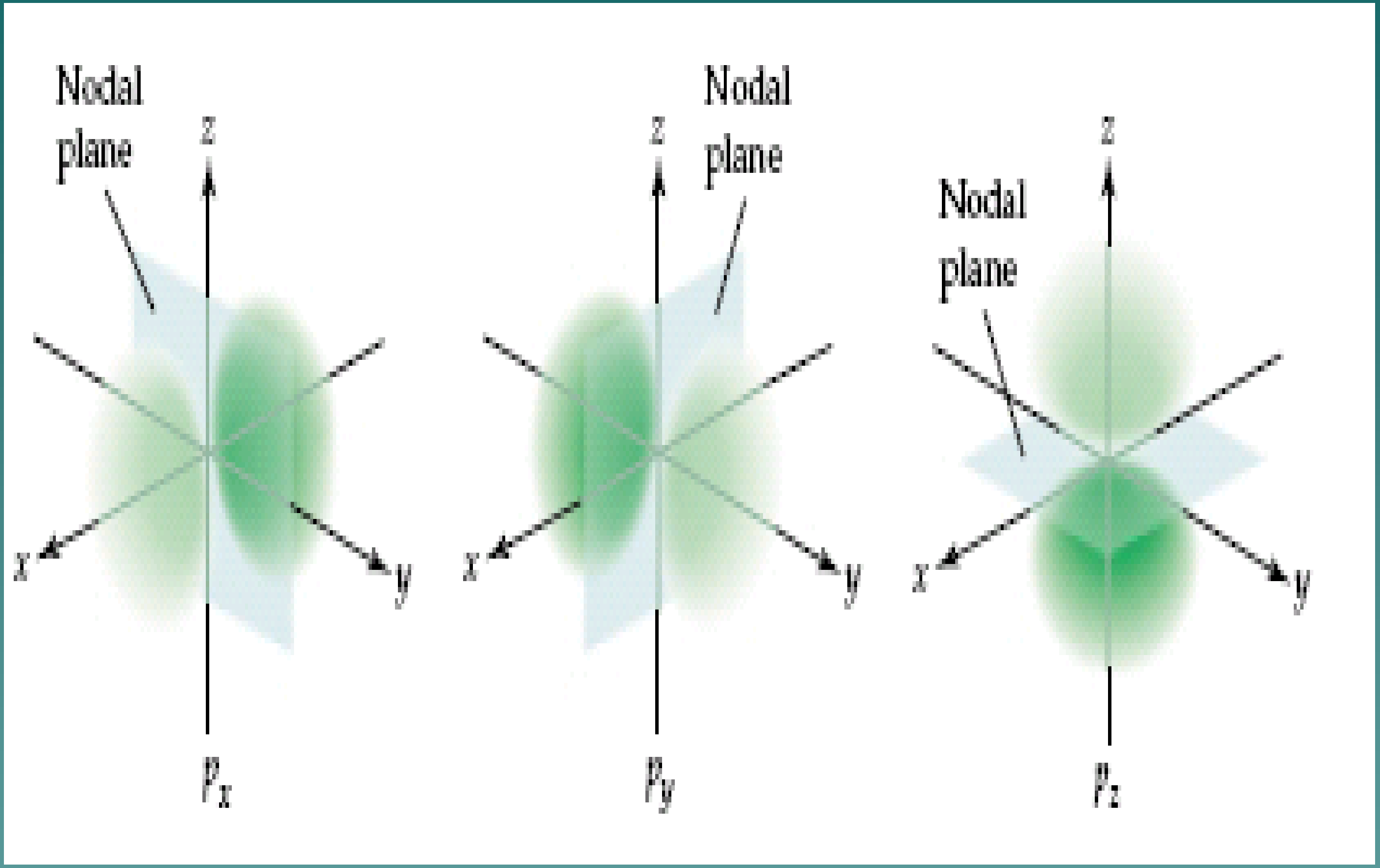
- L=0 (s) orbitals
- L=1 (p) orbitals
- L=2 (d) orbitals
- L=3 (f) orbitals

Quantum number l:	0	1	2	3	4 …
Subshell notation:	s	p	d	f	g …

- For hydrogen and other one-electron atoms, such as(He^+) the energy of an orbital depends *only* on *n*. For atoms with more than one electron, the energy level of an orbital depends both on *n* and on the *l* quantum number

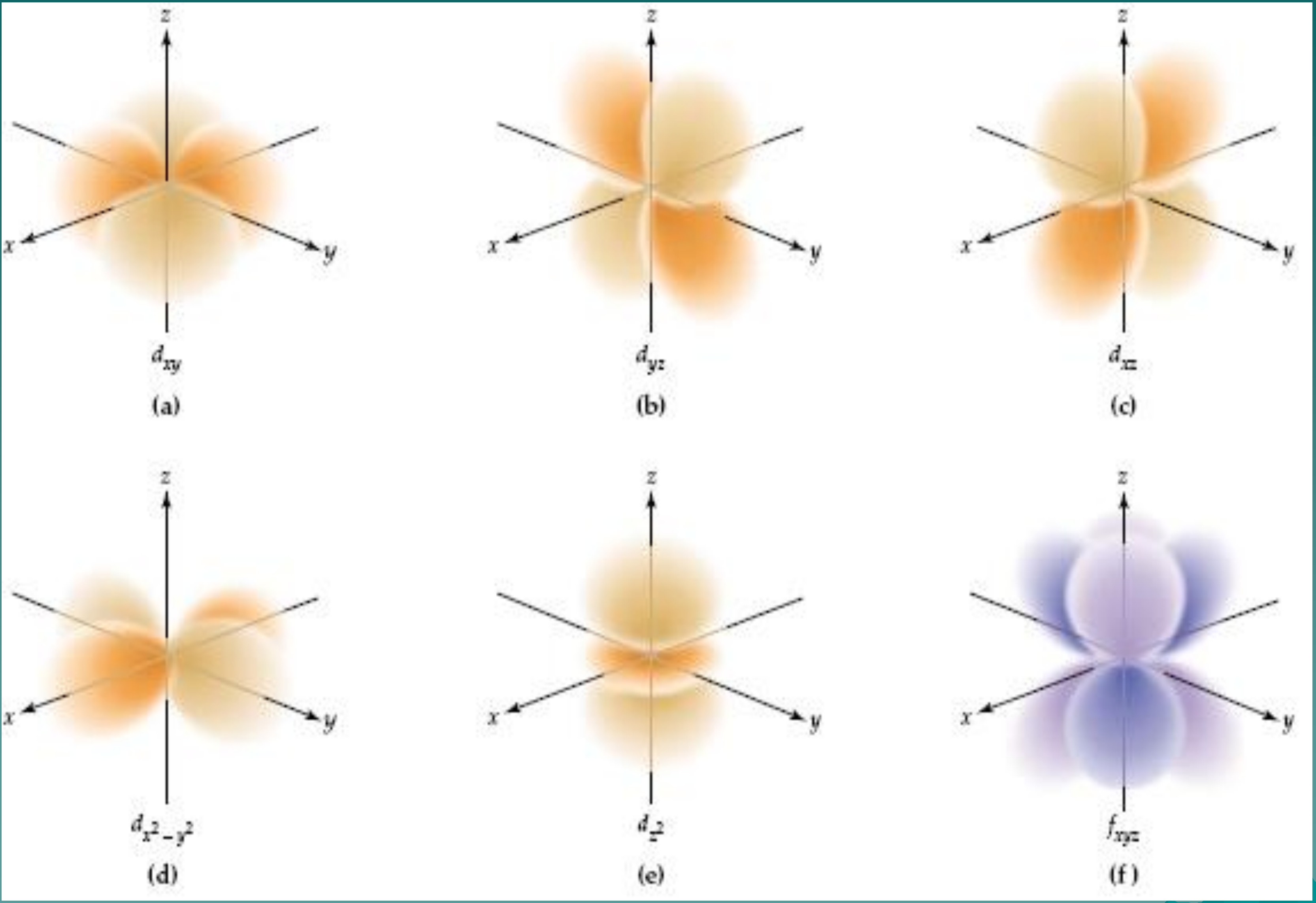

Node
Node
(a)
(b)
(c)

- **FIGURE(1) Representations of (a) 1*s*, (b) 2*s*, and (c) 3*s* orbitals.**
- **As the value of *n* increases, the number of allowed orbitals increases and the size of those orbitals becomes larger, thus allowing an electron to be farther from the nucleus. Because it takes energy to separate a negative charge from a positive charge, this increased distance between the electron and the nucleus means that the energy of the electron in the orbital increases as the quantum number *n* increases.**



Nodal plane
z
x
y
p_x
Nodal plane
z
x
y
p_y
Nodal plane
z
x
y
p_z

- **FIGURE 2**
- Representations of the three 2*p* orbitals, each of which is dumbbell-shaped and oriented in space along one of the three coordinate axes *x*, *y*, or *z*. Each *p* orbital has two lobes of high electron probability separated by a nodal plane passing through the nucleus


z
x
y
d_{xy}
(a)
d_{yz}
(b)
d_{xz}
(c)
$d_{x^2-y^2}$
(d)
d_{z^2}
(e)
f_{xyz}
(f)

- **FIGURE 3**
- Representations of the five 3*d* orbitals. Four of the orbitals are shaped like a cloverleaf **(a–d)**, and the fifth is shaped like an elongated dumbbell inside a donut **(e)**. Also shown is one of the seven 4*f* orbitals **(f)**. As with *p* orbitals in Figure 5.12, the different shadings of the lobes reflect different phases

- The s orbital is spherical with the nucleus at the center of the sphere.
- The other orbitals have point with zero probability of finding an electron these are called nodes.
- P and d orbitals have directional properties by virtue of their orientation along axes in three – dimensional space

- The end