University of karbala
Lec: Two
Collage of pharmacy

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Course title: Inorganic medicinal and Pharmaceutical Chemistry.

- **Lec Title: Electronic structure of atoms: (part two)**

The magnetic quantum number

$-l$ to $+l$.

- defines the spatial orientation of the orbital with respect to a standard set of coordinate axes .

- For an orbital whose angular-momentum quantum number is *l*, the magnetic quantum number ml can have any integral value from to Thus, within each sub shell (orbitals with the same shape, or value of *l*), there are different spatial orientations for those orbitals

If $l = 0$, then $m_l = 0$

If $l = 1$, then $m_l = -1, 0, \text{or } +1$

If $l = 2$, then $m_l = -2, -1, 0, +1, \text{or } +2$

. . . and so forth

- A summary of the allowed combinations of quantum numbers for the first
- four shells is given in Table (1)

n	l	m_l	Orbital Notation	Number of Orbitals in Subshell	Number of Orbitals in Shell
1	0	0	1*s*	1	1
2	0	0	2*s*	1	4
	1	−1, 0, +1	2*p*	3	
3	0	0	3*s*	1	9
	1	−1, 0, +1	3*p*	3	
	2	−2, −1, 0, +1, +2	3*d*	5	
4	0	0	4*s*	1	16
	1	−1, 0, +1	4*p*	3	
	2	−2, −1, 0, +1, +2	4*d*	5	
	3	−3, −2, −1, 0, +1, +2, +3	4*f*	7	

4-The spin quantum Number :

- This number is presented by the symbol (ms) the electron can be envisioned in its particle state as a spinning mass. Since it is charged it will have a magnetic moment +1/2 ,–1/2. These are the only two allowed values of m_s .

- The significance of this is that for two electrons to occupy the same orbital they must have opposing spin if one has +1/2 the other must have,–1/2.

The aufbau process :

- **The aufbau process :**
- This process of atom build the fundamental rules that must be follows the first is.

1-pauli Exclusion principle

- 1-pauli Exclusion principle: it states that in any atom no two electrons may be described by the same set of values for the four quantum numbers

Ex : **two electron in an orbital** .

- (n) is the same
- (l) is the same
- (ml) is the same and ms +1/2 ,-1/2 other rules which apply to describe processes are :

Hands rule:

- In the ground state of any atom ,an electron may enter only the vacant orbital of lowest or lower energy orbitals must be filled before.
- Electrons must enter degenerate orbitals that is orbitals have the same energy .
- Ex 2px ,2py ,2pz so these electrons should enter singly with parallel spin. Or electrons should remain un paired in degenerate orbitals as long as possible.

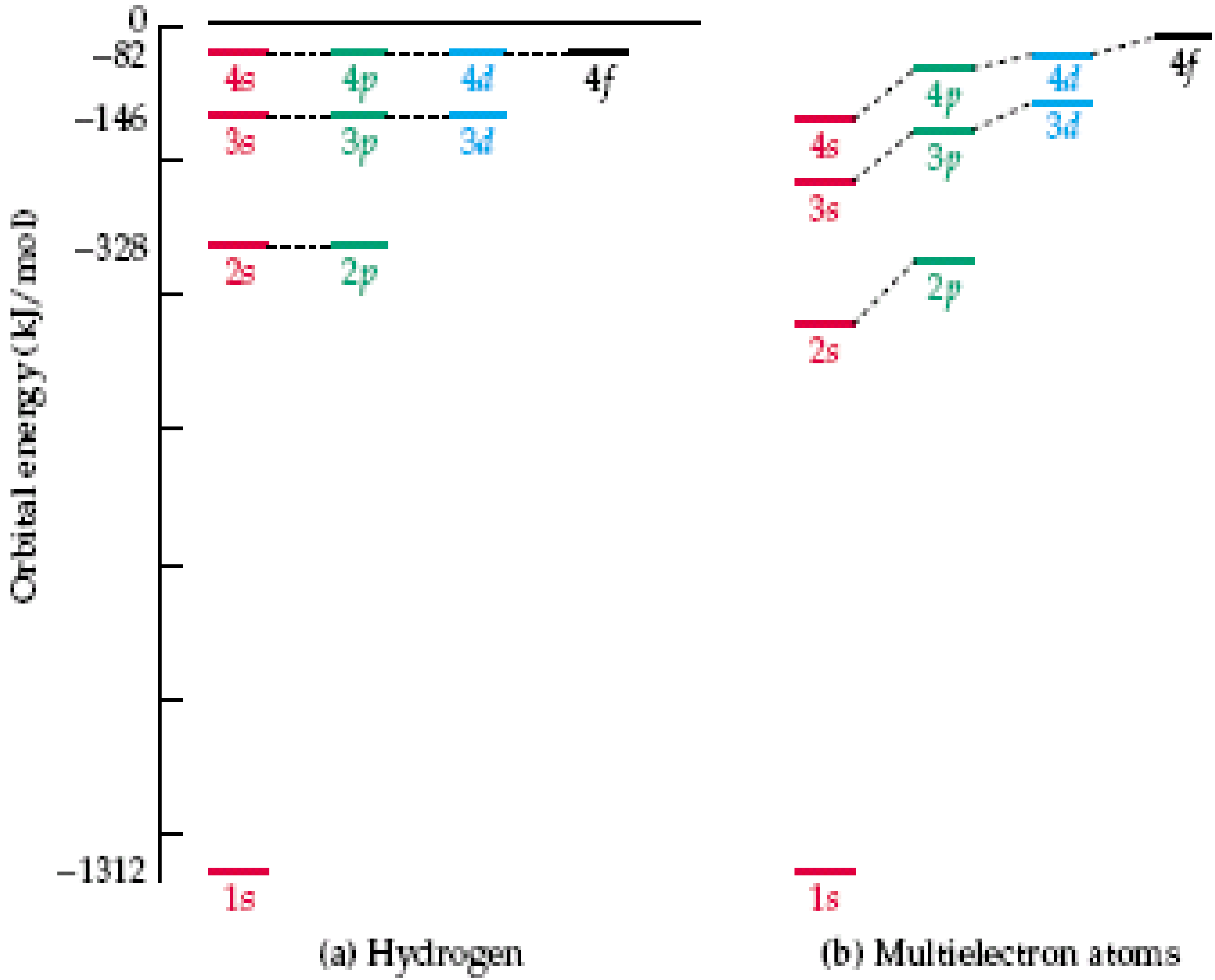
- It will be noticed that the electronic configuration of most atoms is the same as the atom having the next lowest atomic number ,with exception of the added electron .

- In moving from atom to atom the correct number of protons and neutron must be present in the nucleus .
- The number of protons is equal to the number and the number of neutrons could be obtained by subtracting atomic number from the atomic mass.

Note should be applied:

- orbitals in the first and second principal quantum number n=1 or n=2 are filled in the order as expected.
- Starting with the third principal quantum number n=3 the ns orbital must be filled before electrons can be added to an (n-1)d orbital Starting with third principal quantum number the (n-1)d orbitals must be filled before the electrons can enter the np orbital

- in elements where f orbital which the low-lying orbital are filled and some atoms will have an electron or two in the next highest d orbital .



0
−82
−146
−328
−1312
Orbital energy (kJ/mol)
4s
4p
4d
4f
3s
3p
3d
2s
2p
1s
(a) Hydrogen
(b) Multielectron atoms

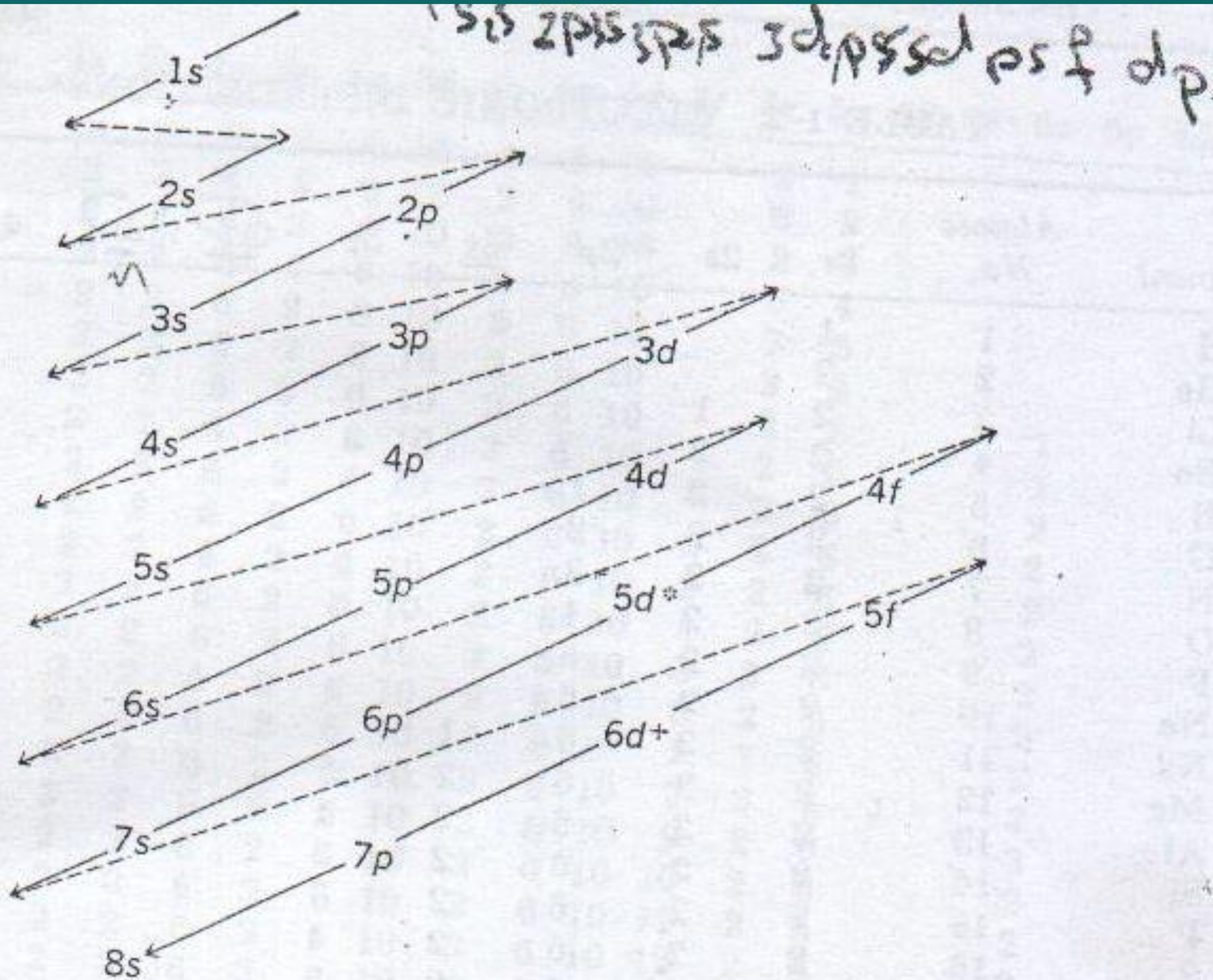


FIG. 1–2. Order of fill

- **FIGURE(1)** Orbital energy levels for (**a**) hydrogen and (**b**) a typical multielectron
- atom. The differences between energies of various subshells in (**b**) are exaggerated for clarity.

- The certain elements in the transition series where d orbital are being filled level will be only half filled and the(n-1 d orbital) will be either half filled or full.

- Ex(1) : Cr chromium At.No.24 has another structure 3d5 4s1
- Ex(2) :Copper At.No.29 has another structure 3d10 4s1

- **As a shorthand means of writing electronic configuration it is possible to used the inert gas (core) that precedes the element being consider.**
- **Ex(1) Na (11) which has the electronic configuration**
- **Na : 1s2 2s2 2p6 3s1 can be written using the Neon core for the first ten electrons**
- **Na [Ne]3s1**
- **Mn(25) [Ar]3d5 4s2**
- **Ne=10 e   Ar=18e .**

- Ionization :
- The process of losing one or more electrons by chemical or physical means is known as ionization and the positive ion produce is termed a cation .
- This process is distinctly different from Aufbau process in that is based in physical reality and should not be taken as the exact opposite of the process of atom build up.

- It is always the most loosely (held) electrons which are lost first when an atom ionizes. However, the electronic structure of ion may not reveal(قد لا يكشف) the level from which the electron was lost. This is particularly true(صحيح بشكل خاص) for the transition elements .

There are several reasons for this

- **This means that a high energy orbitals in one atom may be of lower energy in neighboring atom.**
- **1-Relative orbital energies are subject) عرضة للتغيير) to change as electrons are placed in them.**
- **2-the possibility of rearrangement of the remaining electrons in an ion to a more stable configuration.**
- **Usually atoms in transition series with incompletely filled d orbitals will ionize to leave d ions.**

- Cobalt(27) would ionized
- Co [Ar] 3d7 $4s^2$
  Co2+ [Ar] 3d7

- But this dose not means that both electron were lost from the 4s orbital.
- one or both electrons may be lost from the 3d orbital followed by rearrangement of all the valence electrons into this orbital

- Atom in which s or p orbitals are being filled will usually ionized to form ions with either gas or expand outer shells.
- Those which form cations with inert gas shell structure include elements like Na and Mg .

Mg[Ne]3s2 → [Mg]2+ [Ne]3s1

$$Na:1s^2 2s^2 2p^6 3s^1 \xrightarrow{-e^-} Na^+:1s^2 2s^2 2p^6$$

PROBLEM 6.1 Predict the ground-state electron configuration for each of the following ions, and explain your answers.

(a) Ra^{2+} (b) La^{3+} (c) Ti^{4+} (d) N^{3-}

PROBLEM 6.2 What doubly positive ion has the following ground-state electron configuration? $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}$

- In periodic table elements with ions having inert gas configuration correspond to the elements in groups IA and IIA and the inert gas shell of the ion is group VIIA of preceding period.

Quiz

- Quiz

- Quiz
- What is the quantum number describe?
- Draw the shape of p orbitals in execs?