Quantum Numbers and Atomic Structure

Chapter 3.5, 3.6 and 3.7

Quantum Mechanical Model

Is the "simplest" equation to calculate the *probability* of finding an electron in hydrogen was developed by Schrödinger (1926).

ORBITAL = *3-dimensional plot of all points in space where the probability of finding the electron is some constant (normally 90%)*.

Quantum numbers are used to define the allowed orbitals and describe the behavior of the electron in the orbital

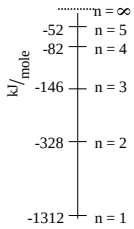
I will expect you to KNOW the following four quantum numbers, their allowed values, and what they represent

Principle Quantum Number *n*

can have any integer value greater than zero; $n = 1, 2, 3, 4 \ldots$

as *n* increases, E increases

also, the *relative* size of the orbital increases with increasing *n* (i.e. the electron is further away from nucleus; can't say anything about radius).



Angular Momentum (Secondary) Quantum Number *l*

l can have integral values from 0 to n-1

e.g.

n	*l*
1	0
2	0,1
3	0,1,2
4	0,1,2,3

also referred to as:

l =	0	1	2	3
	s	p	d	f

the value of *l* determines the shape of an orbital

the energy of the orbital depends on *l* only in a multi-electron case; for electrons with same *n*, energy of $l = 1 < l = 2 < l = 3$ ...

Magnetic Quantum Number m_l

all integer values from $-l$ to $+l$, including 0

l	m_l
0	0
1	-1, 0, +1
2	-2, -1, 0, +1, +2

also known as directional quantum number

distinguishes between orbitals with same shape and energy, but which are oriented in different directions.

energy of the electron is NOT affected by m_l

Spin Quantum Number m_s

values of $+1/2$ (NOT dependent on *n*, *l*, or m_l)

identifies an electron in an orbital (max. 2)

arbitrary: $+1/2$ "spin up" ↑

$-1/2$ "spin down" ↓

Arrangement of Electrons in Atoms

Electrons in atoms are arranged as

SHELLS (Energy Level) (n)

↓

SUBSHELLS (Sublevels) (l)

↓

ORBITALS (Orientation) (m_l)

Quantum Review

Principle quantum number
n = 1, 2, 3,….. **describes orbital size and energy**

Angular momentum quantum number
l = 0 to n-1 **describes orbital shape**

Magnetic quantum number
m_l = l, -1…+1 **describes orientation in space of the orbital relative to the other orbitals in the atom**

Spin quantum number
m_s = +1/2 or -1/2 **describes the direction of spin of the e^- on its axis**

Pauli Exclusion Principle: "no two electrons in an atom can have the same set of quantum numbers", or, only two electrons (of opposite spin) per orbital.

Learning Check: Are These Valid Sets of Quantum Numbers?

(n, l, m_l, m_s)

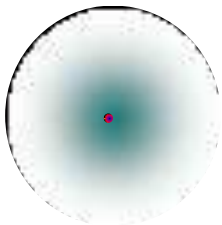
- (1,0,1/2,1/2)
- (3,0,0,+1/2)
- (2,2,1,+1/2)
- (4,3,-2,+1/2)
- (3,2,1,1)

- List all the possible subshells and orbitals associated with the principal quantum number **n** if **n** =5. Indicate the number of electrons as you go.
- Which of these sets of quantum numbers describes an electron in a *4p* orbital?
  (4,2,2,1/2); (3,1,0,-1/2); (4,1,-1,1/2)
- Write the four quantum numbers for an electron in a *5p* orbital.

Shapes of Orbitals

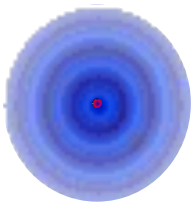
s Orbital

Spherical



Shapes of Orbitals

s Orbitals
Can have several radial maxima



Shape and Location of the Orbitals

A given set of quantum numbers completely characterizes the shape, size, and orientation of an orbital

n : higher values mean that the region of highest probability for the electron is further from the nucleus; i.e. 3s > 2s > 1s

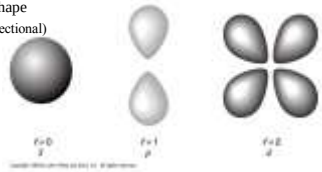
l : defines orbital shape:

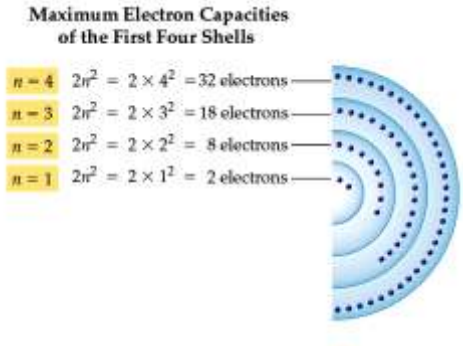
l = 0 s-orbital spherical shape

m_l = 0 (sphere's are not directional)

1 s-orbital

l = 1 p-orbital 2 lobes

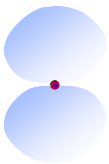




Shapes of Orbitals

p orbital

Dumbbell



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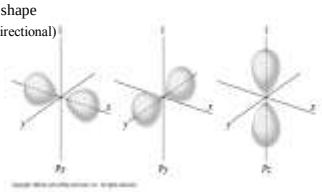
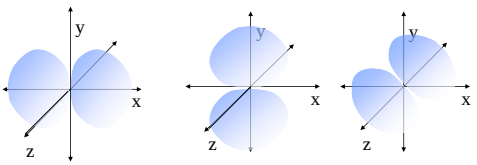
3 p-orbitals: p_x p_y p_z



3 Sets of p Orbitals



p_x p_y p_z

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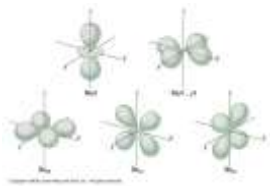
m_l = -1, 0, +1

3 p-orbitals: p_x p_y p_z

l = 2 d-orbital 4 lobes

m_l = -2, -1, 0, +1, +2

5 d-orbitals: d_{xy} d_{xz} d_{yz} $d_{x^2-y^2}$ d_{z^2}



Shapes of Orbitals

d orbital

Shape and Location of the Orbitals

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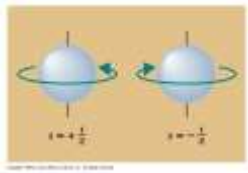
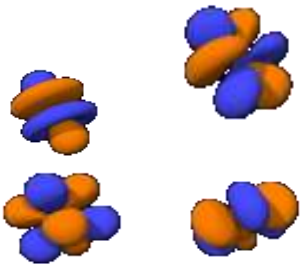
l : defines orbital shape:

- *l* = 0 s-orbital spherical shape
  - m_l = 0 (sphere's are not directional)
  - 1 s-orbital
- *l* = 1 p-orbital 2 lobes
  - m_l = -1, 0, +1
  - 3 p-orbitals: p_x p_y p_z
- l = 2 d-orbital 4 lobes
  - m_l = -2, -1, 0, +1, +2
  - 5 d-orbitals: d_{xy} d_{xz} d_{yz} $d_{x^2-y^2}$ d_{z^2}

m_s : $^1/_2$, each orbital can hold 2 electrons

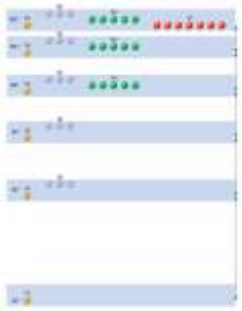


Shapes of Orbitals

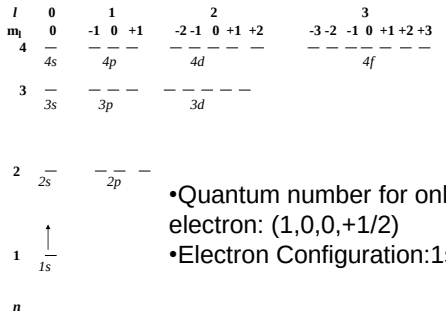


F orbital

Relative Orbital Energies

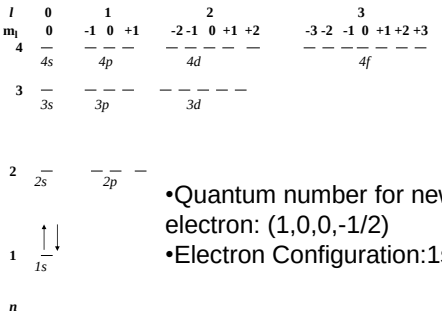


Energy Level Diagram for Hydrogen



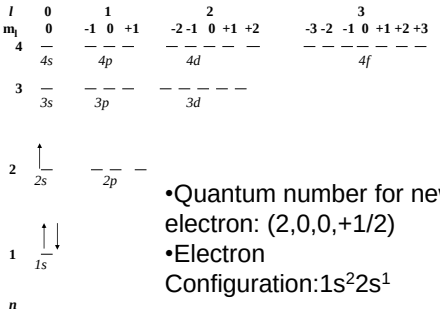
- Quantum number for only electron: (1,0,0,+1/2)
- Electron Configuration:$1s^1$

Energy Level Diagram for Helium



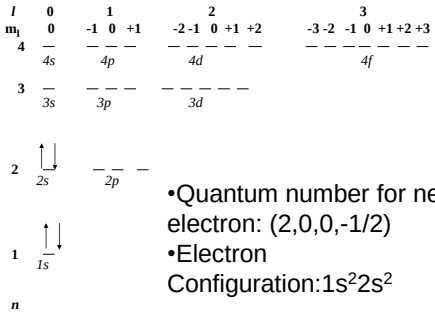
- Quantum number for new electron: (1,0,0,-1/2)
- Electron Configuration:$1s^2$

Energy Level Diagram for Lithium



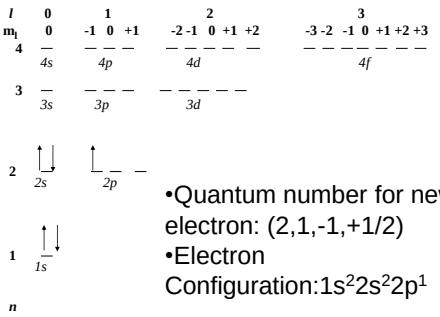
- Quantum number for new electron: (2,0,0,+1/2)
- Electron Configuration: $1s^2 2s^1$

Energy Level Diagram for Beryllium



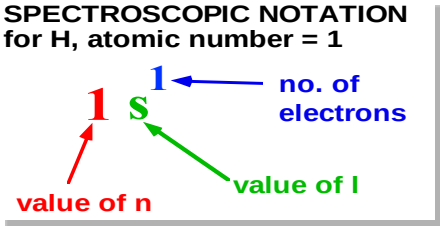
- Quantum number for new electron: (2,0,0,-1/2)
- Electron Configuration: $1s^2 2s^2$

Energy Level Diagram for Boron



- Quantum number for new electron: (2,1,-1,+1/2)
- Electron Configuration: $1s^2 2s^2 2p^1$

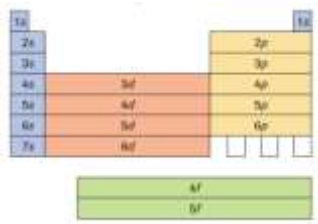
Writing Atomic Electron Configurations



Ways of Expressing Electronic Configurations

- Full configuration
  - Complete ordered placement starting with $1s^2$
    - $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^4$
    - $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^2$
- Condensed configuration
  - Completed noble gas configuration in brackets followed by detail for unfilled valence shell
    - $[Ar]\ 4s^2\ 3d^4$
    - $[Ar]\ 4s^2\ 3d^{10}\ 4p^2$
- Orbital diagrams for outer valence shell
  - Labeled picture of outer valence shell
  - P = [Ne] ↓↑ ↓ ↓ ↓ (3s: ↓↑; 3p: ↓ ↓ ↓)

Periodic Blocks



Rules for Placing Electrons

- Hund's rule
  - Electrons are placed in individual orbitals before being paired up
    - Minimize repulsions
- Overlapping Energy levels
  - 4s is lower in energy than 3d (and 5s is lower than 4d, etc)
  - **Follow the order in the Periodic Table!!**
- Exceptions to "normal" order
  - Cr (half filled 3d and half filled 4s)
  - Cu (complete 3d and half filled 4s)
  - Not responsible!

- Exercise in placing electrons 1
  http://wine1.sb.fsu.edu/chm1045/notes/Struct/EConfig/Struct08.htm
- Exercise in placing electrons 2
  http://wine1.sb.fsu.edu/chm1045/notes/Struct/EPeriod/Struct09.htm
- Electron shells – pages 1 to 7
  http://www.chem.ox.ac.uk/vrchemistry/8eChemistry/html/page01.htm

Electron Filling Order