Republic of Iraq
Ministry of Higher Education & Scientific research
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Introduction in Chemistry

For

First Year Student

Lecture 4

By

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Quantum Number

An atomic orbital is specified by four quantum numbers. These determine the orbital's size, shape, and orientation in the space of orbital.

1- **The principal quantum number (n)** tells the average relative distance of an electron from the nucleus, and the energy of the electron in an atom. (It can have only positive integer n= 1,2,3,4,…..). The larger the value of n, the higher energy and the larger orbital, or electron shell.

2- **The angular momentum quantum number (ℓ)** or orbital quantum number describes the shape of the orbital, and the shape is limited by the principal quantum number n (the shape of the region of space occupied by the electron), (ℓ= 0, 1, 2, 3, …… n-1).

- **Notice;** the value of l defines the shape of the orbital, and the value of n defines the size.
- **Notice;** Orbitals that have the same value of n but different values of ℓ are called subshells. These subshells are given different letters to help chemists distinguish them from each other.
- For example **ℓ= 0, 1, 2, 3**
- **Name = s, p, d, f**

3- **The magnetic quantum number (mℓ)** represents the orientation of the region in space occupied by an electron with respect to an applied magnetic field. (The value of mℓ depends on the value of **ℓ, mℓ**= +l , 0 , l).

4- **Spin Quantum Number(ms):** of the spin axis of an electron, either clockwise or counter-clockwise. Only two values are allowed for ms +1/2 and -1/2 .

- **Notice;** the maximum number of electrons may the atomic subshell contains calculated by the relation $[2 \times (2\ell + 1)]$.

Subshells

The number of values of the orbital angular number ℓ can also be used to identify the number of subshells in a principal electron shell:

- When $n = 1$, $\ell = 0$ (l takes on one value and thus there can only be one subshell)
- When $n = 2$, $\ell = 0, 1$ (l takes on two values and thus there are two possible subshells)
- When $n = 3$, $\ell = 0, 1, 2$ (l takes on three values and thus there are three possible subshells)
- After looking at the examples above, we see that the value of n is equal to the number of subshells in a principal electronic shell:

1. Principal shell with $n = 1$ has one s subshell ($\ell = 0$)
2. Principal shell with $n = 2$ has one s subshell and one p subshell ($\ell = 0, 1$)
3. Principal shell with $n = 3$ has one s subshell, one p subshell, and one d subshell ($\ell = 0, 1, 2$)

We can designate a principal quantum number, n, and a certain subshell by combining the value of n and the name of the subshell (which can be found using ℓ). For example, 3p refers to the third principal quantum number ($n=3$) and the p subshell ($\ell =1$).

n	*l*	*ml*	ms	Number of orbitals	Orbital Name	Number of electrons	Total Electrons
1 (K shell)	0	0	½ - ½	1	1*s*	2	2
2 (L Shell)	0	0	½ - ½	1	2*s*	2	8
	1	-1, 0, +1	½ - ½	3	2*p*	6	
3 (M-shell)	0	0	½ - ½	1	3*s*	2	18
	1	-1, 0, +1	½ - ½	3	3*p*	6	
	2	-2, -1, 0, +1, +2	½ - ½	5	3*d*	10	
4 (L-shell)	0	0	½ - ½	1	4*s*	2	32
	1	-1, 0, +1	½ - ½	3	4*p*	6	
	2	-2, -1, 0, +1, +2	½ - ½	5	4*d*	10	
	3	-3, -2, -1, 0, +1, +2, +3	½ - ½	7	4*f*	14	

Quantum Number Chart

Example: Give the name, magnetic quantum numbers, and number of orbitals for each sublevel with the given n and l quantum numbers: (a) n = 3, ℓ = 2 (b) n = 2, ℓ= 0 (c) n = 5, ℓ = 1 (d) n = 4, ℓ = 3 Solution:

	n	ℓ	Subshell name	Possible ml	No.of orbtal
a	3	2	3d	+2,+1,0,-1,-2	5
b	2	0	2S	0	1

c	5	1	5p	+1,0,-1	3
d	4	3	4f	+3,+2,+1,0,-1,-2,-3	7

Problem: What is wrong with each of the following quantum number designations and/or subshell names?

	n	ℓ	ml	Name
a	1	1	0	1p
b	4	3	+1	4d
c	3	1	-2	3p

Solution:

(a) A sublevel of n = 1 can have only ℓ = 0, not ℓ = 1. The only possible subshell is 1s.

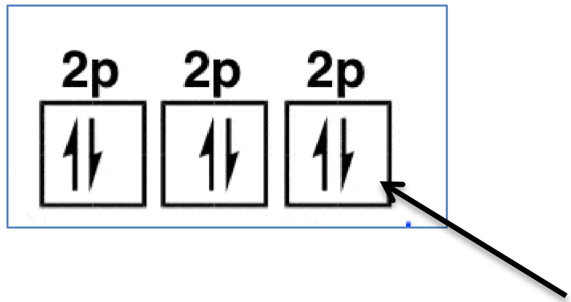
(b) A subshell with ℓ= 3 is an f subshell, not a d subshell. The subshell name should be 4f.

c) A subshell with ℓ= 1 can have only mℓ of -1, 0, +1, not -2.

Example: Write a set of quantum numbers for the last electrons in ground state and ions in a Ne atom.

Ne =$1s^2\ 2s^2\ 2p^6$

n = 2, ℓ = 1, mℓ= -1, ms = -1/2



Last electron

***no ions for noble gas**

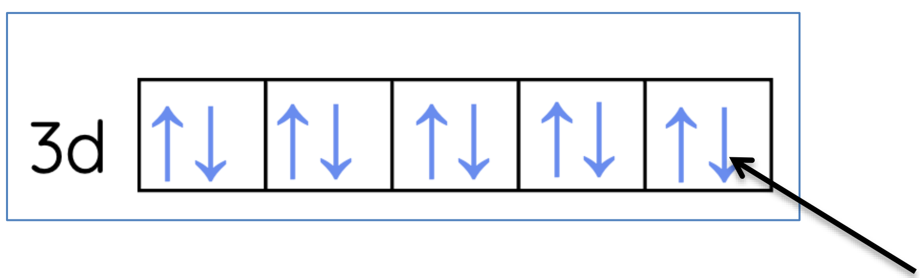
Example: Give the value for all four quantum number for the last electron in the ground state of Cu_{29}.

solution

Cu_{29} :$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^9$

Cu_{29} : $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^1$

n= 3, ℓ= 2, mℓ = -2, ms= -1/2



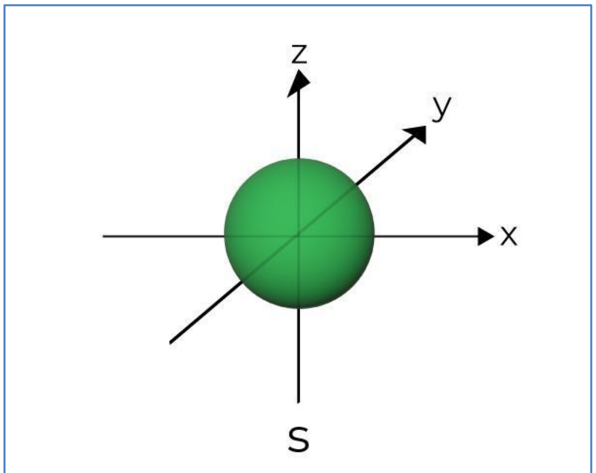
Last electron

Atomic Orbital Shapes

Size of orbitals; defined as the surface that contains 90% of the total electron probability.

S Orbital

S orbitals are spherical with the nucleus at the center. When n increases, s orbitals become larger and higher in energy because of their increased distance from the nucleus. Note: Each subshell of the H atom has orbitals with a characteristic shape. s orbitals (l = 0) are spherically symmetrical around the nucleus.



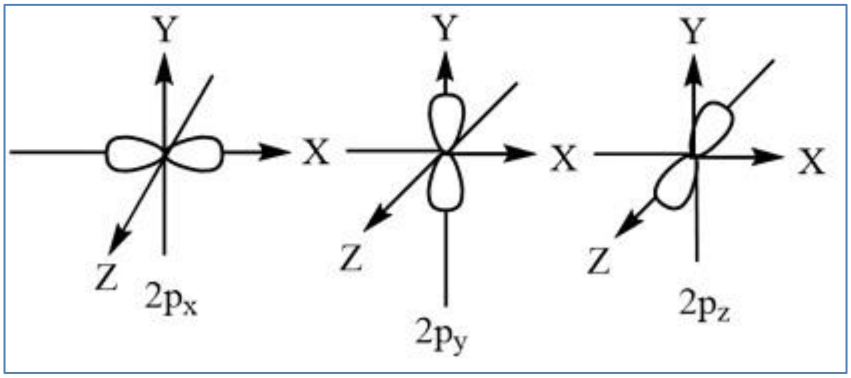
Shape of s-orbital

P Orbitals

There are three P orbitals in each P subshell, occur in levels n=2 and greater. All P orbitals have the same basic shape (two lobes arranged along a straight line with the nucleus between the lobes)but differ in their orientations in space). We denote these orbitals as 2Px, 2Py, and 2Pz. A 2Px orbital has its greatest electron probability along the x-axis, a 2Py orbital along the y-axis, and a 2Pz orbital along the z-axis.

Notice;

as the value of l increases, the number of orbitals in a given subshell increases, and the shapes of the orbitals become more complex. Energies of p orbitals: 2p < 3p < 4p.



d Orbitals

Occur in levels n = 3 and greater. Two fundamental shapes; a. Four orbitals with four lobes for each one, centered in the plane indicated in the orbital label dxz, dyz, dxy, and $dx^2 - y^2$ b. Fifth orbital is uniquely shaped - two lobes along the z-axis and a belt centered in the xy plane dz^2.