

❖ Quantum Numbers

1- Principal Quantum Number(n):

$n = 1, 2, 3, \dots, \infty$. Specifies the energy of an electron and the size of the orbital (the distance from the nucleus to orbital). All orbitals that have the same value of n are said to be in the same shell (level). For a hydrogen atom with $n=1$, the electron is in its **ground state**; if the electron is in the $n=2$ orbital, it is in an **excited state**. The total number of **orbitals** for a given n value is n^2 . The total number of electron for a given n value is $2n^2$.

2- Angular Momentum (Secondary or Azimunthal) Quantum Number (l):

$l = 0, 1, 2, \dots, (n-1)$. Specifies the **shape** of an orbital with a particular principal quantum number. The secondary quantum number divides the shells into smaller groups of orbitals called **subshells (sublevels)**. Usually, a letter code is used to identify l to avoid confusion with n :

l	0	1	2	3	4	5	...
Letter	<i>s</i>	<i>p</i>	<i>d</i>	<i>f</i>	<i>g</i>	<i>h</i>	...

The subshell with $n=2$ and $l=1$ is the **2p subshell**; if $n=3$ and $l=0$, it is the **3s subshell**, and so on. The value of l also has a slight effect on them energy of the subshell; the energy of the subshell increases with l (**s < p < d < f**).

* The value of l determines not only the shape of an orbital but also the amount of orbital angular momentum associated with an electron in it:

$$\text{Orbital angular momentum} = \left[\sqrt{l(l+1)} \right] \frac{h}{2\pi}$$

* An electron in an **s** orbital ($l=0$) has no orbital angular momentum, an electron in a **p** orbital ($l=1$) has angular momentum equal to;

$$\sqrt{2} \left(\frac{h}{2\pi} \right)$$

And so on. The orbital angular momentum vector has $(2l+1)$ possible directions in space corresponding to the $(2l+1)$ possible values of (m_l) for a given value of l .

3- Magnetic Quantum Number (m_l):

$m_l = -l, \dots, 0, \dots, +l$. Specifies the *orientation of orbital in space* or (the orientation of the angular momentum vector in a magnetic field). This number divides the subshell into individual **orbitals** which hold the electrons; there are $2l+1$ orbitals in each subshell. Thus the *s* subshell has only *one* orbital, the *p* subshell has *three* orbitals, and so on.

4- Spin Quantum Number(m_s):

$m_s = +\frac{1}{2}$ or $-\frac{1}{2}$. Determines the orientation of the electron's magnetic moment in a magnetic field, either in the direction of the field $+\frac{1}{2}$ or opposed to it $-\frac{1}{2}$. An electron can spin in only one of two directions (sometimes called *up* and *down*).

❖ 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:

- Principal shell with $n = 1$ has one subshell
- Principal shell with $n = 2$ has two subshells
- Principal shell with $n = 3$ has three subshells

To identify what type of possible subshells n has, these subshells have been assigned letter names. The value of ℓ determines the name of the subshell:

Name of Subshell	Value of (ℓ)
s subshell	0
p subshell	1
d subshell	2
f subshell	3

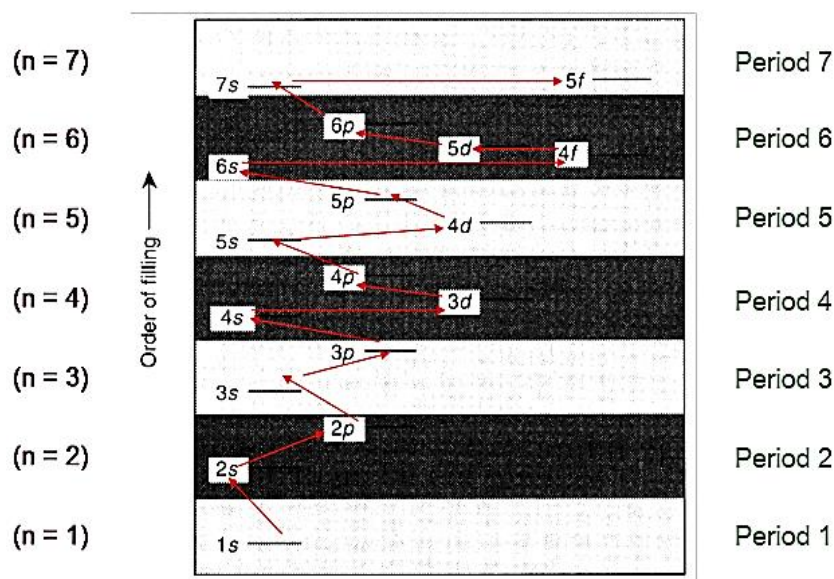
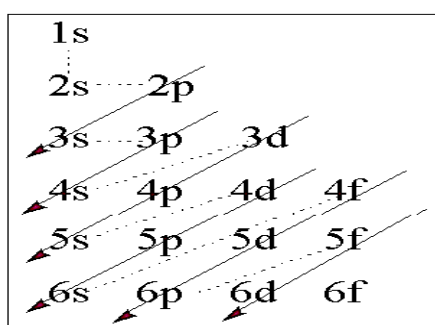
Therefore:

- Principal shell with $n = 1$ has one **s** subshell ($\ell = 0$)

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

❖ Arrangement Of Electrons In Atoms



* In different atoms the filling of electrons into the orbitals takes place according to the three main principles naming the **Aufbau Principle**, **Pauli Exclusion Principle**, and **Hund's rule** of maximum multiplicity:

***Aufbau principle**

- The Aufbau Principle is basically a German word “*Aufbauen*” which means *building up*.
- According to this principle, the **electrons will first occupy the orbitals that have the lowest energy**. This means that the electrons enter first orbital and then enter the orbitals which have higher energy but only when the lower- energy orbitals are completely filled.
- The order in which the electrons should be filled is **1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p**.....
- The order of the increasing energy of the orbitals can also be calculated using $(n+l)$ rule.
- The sum of the values of the principal quantum numbers (**n**) and azimuthal quantum number (**l**) is used to decide the energy level of an orbital.
- The lower value of the sum of $(n+l)$ means that the energy of the orbital is low. If the value of $(n+l)$ for two orbitals is equal then the orbital with a lower value of n will have a lower energy level.

n	l	(n + l)	State
1	0	1	1s
2	0	2	2s
2	1	3	2p
3	0	3	3s
3	1	4	3p
4	0	4	4s
3	2	5	3d
4	1	5	4p
5	0	5	5s
4	2	6	4d
5	1	6	5p
6	0	6	6s
4	3	7	4f
5	2	7	5d
6	1	7	6p
7	0	7	7s

^aIn general, energy increases in going down in the table.

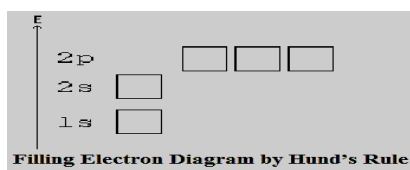
*Pauli Exclusion Principle

- According to this principle, an orbital can have maximum two electrons and these must have opposite spins.
- In other words, states that *no two electrons in the same atom can have identical values for all four of their quantum numbers*. What this means is that no more than **two** electrons can occupy the same orbital, and that two electrons in the same orbital must have **opposite spins**, different m_s values (different spins = spin-paired).
- As we know that fourth quantum number is m_s , $+1/2$ is spin up and $-1/2$ is spin down and hence if the first three quantum numbers are same for two electrons then the electrons must have opposite spins in an orbital

* Hund's rule

- According to this rule, the electrons are filled in the degenerate orbitals of the same subshell.
- **Hund's** first rule (often referred to simply as Hund's rule): in a set of degenerate orbitals, electrons may not be spin-paired in an orbital until each orbital in the set contains one electron; electrons singly occupying orbitals in a degenerate set have parallel spins, i.e. they have the same values of m_s .
- **Electron pairing in p, d, and f orbitals cannot be done until each sub-shell is occupied singly.**
- This is because electrons are the same in charge and they repel each other. This repulsion is minimized if two electrons move away from each other by getting different degenerate orbitals.

- All the orbitals which are singly occupied have parallel spins which can be either clockwise or anticlockwise.



*The tables below represent the electron configuration of elements

Element	Z	Configuration
H	1	1s ¹
He	2	1s ²
Li	3	[He] 2s ¹
Be	4	[He] 2s ²
B	5	[He] 2s ² 2p ¹
C	6	[He] 2s ² 2p ²
N	7	[He] 2s ² 2p ³
O	8	[He] 2s ² 2p ⁴
F	9	[He] 2s ² 2p ⁵
Ne	10	[He] 2s ² 2p ⁶
Na	11	[Ne] 3s ¹
Mg	12	[Ne] 3s ²
Al	13	[Ne] 3s ² 3p ¹
Si	14	[Ne] 3s ² 3p ²
P	15	[Ne] 3s ² 3p ³
S	16	[Ne] 3s ² 3p ⁴
Cl	17	[Ne] 3s ² 3p ⁵
Ar	18	[Ne] 3s ² 3p ⁶
K	19	[Ar] 4s ¹
Ca	20	[Ar] 4s ²
Sc	21	[Ar] 4s ² 3d ¹
Ti	22	[Ar] 4s ² 3d ²
V	23	[Ar] 4s ² 3d ³
Cr	24	* [Ar] 4s ¹ 3d ⁵
Mn	25	[Ar] 4s ² 3d ⁵
Fe	26	[Ar] 4s ² 3d ⁶
Co	27	[Ar] 4s ² 3d ⁷
Ni	28	[Ar] 4s ² 3d ⁸
Cu	29	* [Ar] 4s ¹ 3d ¹⁰
Zn	30	[Ar] 4s ² 3d ¹⁰
Ga	31	[Ar] 4s ² 3d ¹⁰ 4p ¹
Ge	32	[Ar] 4s ² 3d ¹⁰ 4p ²
As	33	[Ar] 4s ² 3d ¹⁰ 4p ³
Se	34	[Ar] 4s ² 3d ¹⁰ 4p ⁴
Br	35	[Ar] 4s ² 3d ¹⁰ 4p ⁵
Kr	36	[Ar] 4s ² 3d ¹⁰ 4p ⁶
Rb	37	[Kr] 5s ¹
Sr	38	[Kr] 5s ²
Y	39	[Kr] 5s ² 4d ¹
Zr	40	[Kr] 5s ² 4d ²
Nb	41	* [Kr] 5s ¹ 4d ⁴
Mo	42	* [Kr] 5s ¹ 4d ⁵
Tc	43	[Kr] 5s ² 4d ⁵
Ru	44	* [Kr] 5s ¹ 4d ⁷
Rh	45	* [Kr] 5s ¹ 4d ⁸
Pd	46	* [Kr] 4d ¹⁰
Ag	47	* [Kr] 5s ¹ 4d ¹⁰
Cd	48	[Kr] 5s ² 4d ¹⁰
In	49	[Kr] 5s ² 4d ¹⁰ 5p ¹
Sn	50	[Kr] 5s ² 4d ¹⁰ 5p ²
Sb	51	[Kr] 5s ² 4d ¹⁰ 5p ³
Te	52	[Kr] 5s ² 4d ¹⁰ 5p ⁴
I	53	[Kr] 5s ² 4d ¹⁰ 5p ⁵
Xe	54	[Kr] 5s ² 4d ¹⁰ 5p ⁶

Element	Z	Configuration
Cs	55	[Xe] 6s ¹
Ba	56	[Xe] 6s ²
La	57	* [Xe] 6s ² 5d ¹
Ce	58	* [Xe] 6s ² 4f ¹ 5d ¹
Pr	59	[Xe] 6s ² 4f ³
Nd	60	[Xe] 6s ² 4f ⁴
Pm	61	[Xe] 6s ² 4f ⁵
Sm	62	[Xe] 6s ² 4f ⁶
Eu	63	[Xe] 6s ² 4f ⁷
Gd	64	* [Xe] 6s ² 4f ⁷ 5d ¹
Tb	65	[Xe] 6s ² 4f ⁹
Dy	66	[Xe] 6s ² 4f ¹⁰
Ho	67	[Xe] 6s ² 4f ¹¹
Er	68	[Xe] 6s ² 4f ¹²
Tm	69	[Xe] 6s ² 4f ¹³
Yb	70	[Xe] 6s ² 4f ¹⁴
Lu	71	[Xe] 6s ² 4f ¹⁴ 5d ¹
Hf	72	[Xe] 6s ² 4f ¹⁴ 5d ²
Ta	73	[Xe] 6s ² 4f ¹⁴ 5d ³
W	74	[Xe] 6s ² 4f ¹⁴ 5d ⁴
Re	75	[Xe] 6s ² 4f ¹⁴ 5d ⁵
Os	76	[Xe] 6s ² 4f ¹⁴ 5d ⁶
Ir	77	[Xe] 6s ² 4f ¹⁴ 5d ⁷
Pt	78	* [Xe] 6s ¹ 4f ¹⁴ 5d ⁹
Au	79	* [Xe] 6s ¹ 4f ¹⁴ 5d ¹⁰
Hg	80	[Xe] 6s ² 4f ¹⁴ 5d ¹⁰
Tl	81	[Xe] 6s ² 4f ¹⁴ 5d ¹⁰ 6p ¹
Pb	82	[Xe] 6s ² 4f ¹⁴ 5d ¹⁰ 6p ²
Bi	83	[Xe] 6s ² 4f ¹⁴ 5d ¹⁰ 6p ³
Po	84	[Xe] 6s ² 4f ¹⁴ 5d ¹⁰ 6p ⁴
At	85	[Xe] 6s ² 4f ¹⁴ 5d ¹⁰ 6p ⁵
Rn	86	[Xe] 6s ² 4f ¹⁴ 5d ¹⁰ 6p ⁶
Fr	87	[Rn] 7s ¹
Ra	88	[Rn] 7s ²
Ac	89	* [Rn] 7s ² 6d ¹
Th	90	* [Rn] 7s ² 6d ²
Pa	91	* [Rn] 7s ² 5f ² 6d ¹
U	92	* [Rn] 7s ² 5f ³ 6d ¹
Np	93	* [Rn] 7s ² 5f ⁴ 6d ¹
Pu	94	[Rn] 7s ² 5f ⁶
Am	95	[Rn] 7s ² 5f ⁷
Cm	96	* [Rn] 7s ² 5f ⁷ 6d ¹
Bk	97	[Rn] 7s ² 5f ⁹
Cf	98	* [Rn] 7s ² 5f ⁹ 6d ¹
Es	99	[Rn] 7s ² 5f ¹¹
Fm	100	[Rn] 7s ² 5f ¹²
Md	101	[Rn] 7s ² 5f ¹³
No	102	[Rn] 7s ² 5f ¹⁴
Lr	103	[Rn] 7s ² 5f ¹⁴ 6d ¹
Rf	104	[Rn] 7s ² 5f ¹⁴ 6d ²
Db	105	[Rn] 7s ² 5f ¹⁴ 6d ³
Sg	106	[Rn] 7s ² 5f ¹⁴ 6d ⁴
Bh	107	[Rn] 7s ² 5f ¹⁴ 6d ⁵
Hs	108	[Rn] 7s ² 5f ¹⁴ 6d ⁶
Mt	109	[Rn] 7s ² 5f ¹⁴ 6d ⁷
Ds	110	* [Rn] 7s ¹ 5f ¹⁴ 6d ⁹
Rg	111	* [Rn] 7s ¹ 5f ¹⁴ 6d ¹⁰
Cn ^a	112	[Rn] 7s ² 5f ¹⁴ 6d ¹⁰