Quantum Numbers

Second Semester

BSc Chemistry

St. Mary’s College, Manarcaud

Quantum Numbers

Introduction:

Quantum numbers are essential tools in understanding the electronic structure of atoms.
They provide valuable information about the energy, spatial distribution, orientation, and spin of electrons.

Quantum numbers are a set of four values that describe specific properties of electrons within an atom.
The four quantum numbers are the

- **principal quantum number (n),**
- **azimuthal quantum number (l),**
- **magnetic quantum number (ml), and**
- **spin quantum number (ms).**

These four quantum numbers provide complete address of an electrons in an atom

Quantum Numbers	Symbol	Possible Values
Principal QN	n	1,2,3,4…..
Azimuthal QN	ℓ	0,1,2,3….(n-1)
Magnetic QN	m	$-\ell$,….,-1,0,1…,ℓ
Spin QN	s	+1/2,-1/2

PRINCIPAL QUANTUM NUMBER

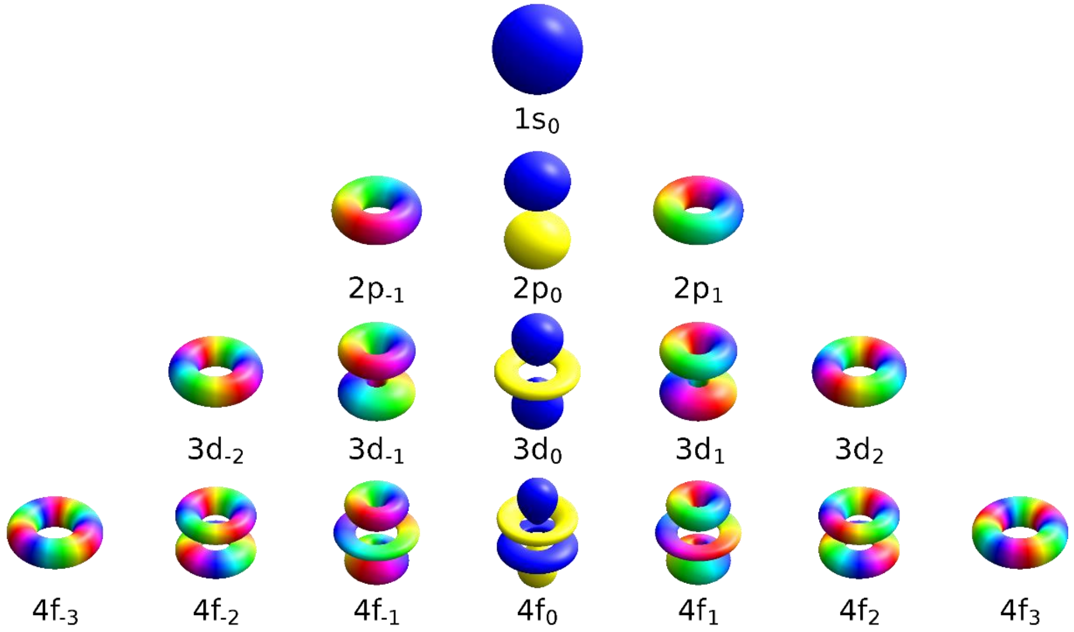
- The principal quantum number (n) defines the energy level or shell in which an electron resides.
- It determines the average distance of an electron from the nucleus and corresponds to the overall size of the orbital.
- Gives the idea about the main energy level to which the electron belongs
- Values: 1, 2, 3, …….. $n = 7$ is the highest number of shell used for the atoms known
- Designated as K,L,M,N etc.
- larger value of the principal quantum number implies a greater distance between the electron and the nucleus.
- The maximum number of electrons possible in a given shell is $2n^2$.

AZIMUTHAL QUANTUM NUMBER(ℓ)

- The azimuthal quantum number (l) describes the shape of an orbital and determines its subshell or sublevel.
- It takes values from 0 to (n-1).
- Each value of l is associated with a specific subshell:
- **0 for s,**
- **1 for p,**
- **2 for d, and**
- **3 for f**.
- The azimuthal quantum number provides information about the orbital's angular momentum and helps visualize different orbital shapes.
- It denotes the sub-shell within the main energy level

- For a given Principal qn (n) It can have values from 0 to (n-1) ie.
- n=1   l = 0   - **1S orbital**
- n=2   l = 0,1- **2S&2P**
- n=3   l = 0,1,2- **3S,3P,3d**

ℓ value	Sub-level	Corresponding spectroscopic terms
0	s-orbital	Sharp
1	p-orbital	Principal
2	d-orbital	Diffuse
3	f- orbital	Fundamental

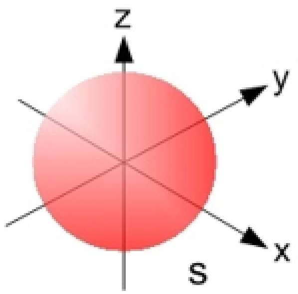


- The energy of the subshell increases with *l* (s < p < d < f).
- The number of electron in a particular subshell is equal to 2(2*l*+1).
- The relationship between orbital angular momentum and azimuthal QN l is
- Angular momentum =$\sqrt{l(l+1)}\,\frac{h}{2\pi}$ = $\sqrt{l(l+1)}\,\boldsymbol{\hbar}$
- For s sub-shell angular momentum *l = o*
- For p sub-shell angular momentum *l* = $\sqrt{2}\,\frac{h}{2\pi}$
- For d sub-shell angular momentum *l* = $\sqrt{6}\,\frac{h}{2\pi}$
- For f sub-shell angular momentum *l* = $\sqrt{12}\,\frac{h}{2\pi}$

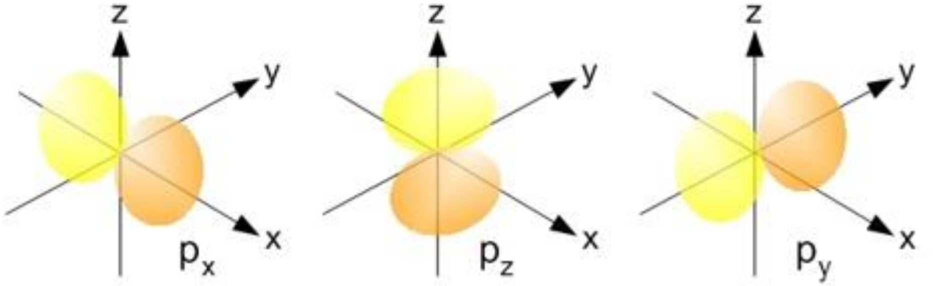
MAGNETIC QUANTUM NUMBER (*m*)

- The magnetic quantum number (m) specifies the orientation of an orbital within a given subshell.
- It takes integer values ranging from -l to +l, including zero.
- For each value of l, there are 2l+1 possible values for m.
- Understanding the magnetic quantum number helps in visualizing the spatial arrangement of orbitals within an atom.
- Denotes the orientation of an electron cloud under the influence of a magnetic field.

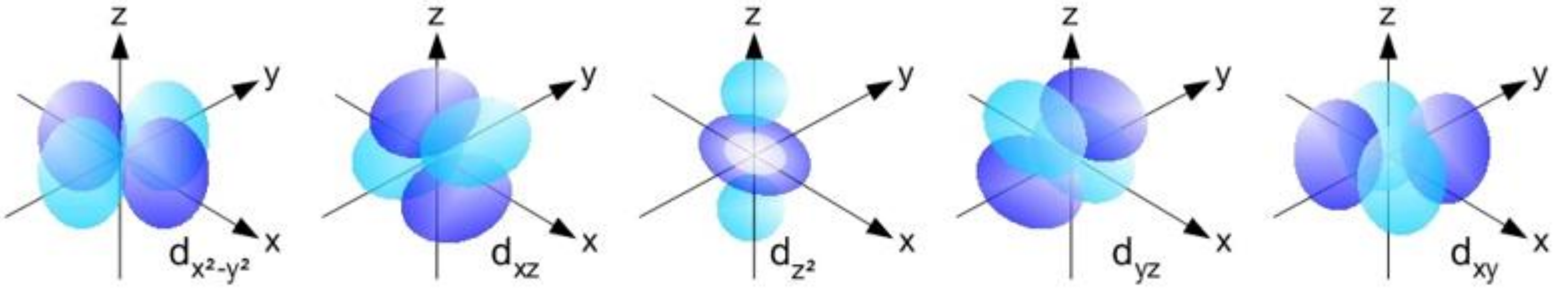
- Magnetic qn m can have values from - l to +l g with a total of 2 l + 1 values
- Total number of values of m in a given value of n = n^2



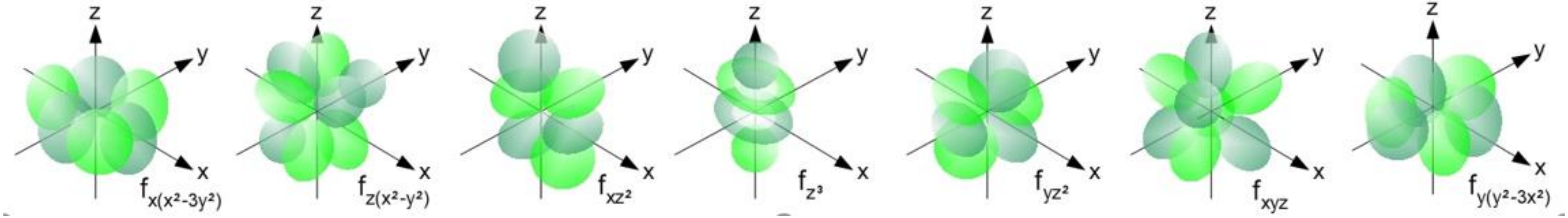
S orbital-l value=0, m value= 0



p orbital-l value=1 m value= -1,0,+1



d orbital-l value=2, m value= -2,-1,0,+1,+2



F orbital -l value=2, m value= -3,-2,-1,0,+1,+2,+3

l Value	State	*m* Values Possible	Maximum Population
0	*s*	0	2
1	*p*	0, ±1	6
2	*d*	0, ±1, ±2	10
3	*f*	0, ±1, ±2, ±3	14
4	*g*	0, ±1, ±2, ±3, ±4	18

Principal quantum number n	Subsidiary quantum number l	Magnetic quantum numbers m	Symbol
1	0	0	1*s* (one orbital)
2	0	0	2*s* (one orbital)
2	1	−1, 0, +1	2*p* (three orbitals)
3	0	0	3*s* (one orbital)
3	1	−1, 0, +1	3*p* (three orbitals)
3	2	−2, −1, 0, +1, +2	3*d* (five orbitals)
4	0	0	4*s* (one orbital)
4	1	−1, 0, +1	4*p* (three orbitals)
4	2	−2, −1, 0, +1, +2	4*d* (five orbitals)
4	3	−3, −2, −1, 0, +1, +2, −3	4*f* (seven orbitals)

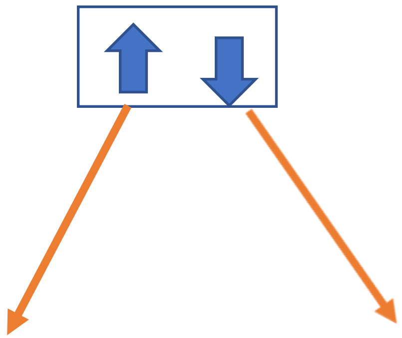
Azimuthal Quantum Number (l)	Magnetic Quantum Number (m_l)	Orbitals
0	0	1s
0	0	2s
1	-1, 0, +1	2px, 2py, 2pz
0	0	3s
1	-1, 0, +1	3px, 3py,3pz
2	-2, -1, 0, +1, +2	3dxz, 3dyz, $3dz^2$, 3dxz, $3dx^2$-y^2
0	0	4s
1	-1, 0, +1	4px, 4py, 4pz
2	-2, -1, 0, +1, +2	4dxz, 4dyz, $4dz^2$, 4dxz, $4dx^2$-y^2
3	-3, -2, -1, 0, +1, +2, +3	$4fx^3$, $4fy^3$, $4fz^3$, 4fxyz, $4fx(y^2-z^2)$, $4fy(z^2-x^2)$, $4fz(x^2-y^2)$

Spin quantum numbers

- The spin quantum number (ms) describes the spin state of an electron.
- It can have two possible values: +1/2 or -1/2, representing the electron's clockwise or counterclockwise spin, respectively.
- The spin quantum number is crucial for understanding electron pairing, magnetic properties, and the Pauli exclusion principle.

Like Magnetic QN *l* , the spin angular quantum number has the magnitude

S=$\sqrt{s(s+1)}\,\frac{h}{2\pi}$



Clock wise spin value-$\frac{+1}{2}$

Anticlockwise spin value- $\frac{-1}{2}$

Total number of orbitals in a main shell

TABLE 6.2 Relationship among Values of n, l, and m_l through $n = 4$

n	Possible Values of l	Subshell Designation	Possible Values of m_l	Number of Orbitals in Subshell	Total Number of Orbitals in Shell
1	0	1*s*	0	1	1
2	0	2*s*	0	1	
	1	2*p*	1, 0, −1	3	4
3	0	3*s*	0	1	
	1	3*p*	1, 0, −1	3	
	2	3*d*	2, 1, 0, −1, −2	5	9
4	0	4*s*	0	1	
	1	4*p*	1, 0, −1	3	
	2	4*d*	2, 1, 0, −1, −2	5	
	3	4*f*	3, 2, 1, 0, −1, −2, −3	7	16

n	Maximum # of electrons($2n^2$)
1	2
2	8
3	18

Maximum number of electrons in a Main shell

Quantum number	Orbital Information	Quantisation of parameters
n	Energy and size of shell	Energy of electron, distance from the nucleus
l	Shape of orbitals(s,p,d,f)	Magnitude of orbital angular momentum
m	Orientation of orbitals in space (number of various types of orbitals)	Direction of orbital angular momentum
s	None	Magnitude and direction of spin angular momentum

Which quantum number describes the overall size of an orbital?
a) Principal quantum number (n)
b) Azimuthal quantum number (l)
c) Magnetic quantum number (ml)
d) Spin quantum number (ms)

Which quantum number determines the shape of an orbital?
a) Principal quantum number (n)
b) Azimuthal quantum number (l)
c) Magnetic quantum number (ml)
d) Spin quantum number (ms)

Which quantum number describes the orientation of an orbital within a subshell?
a) Principal quantum number (n)
b) Azimuthal quantum number (l)
c) Magnetic quantum number (ml)
d) Spin quantum number (ms)

Which quantum number describes the spin state of an electron?
a) Principal quantum number (n)
b) Azimuthal quantum number (l)
c) Magnetic quantum number (ml)
d) Spin quantum number (ms)

What is the maximum number of electrons that can occupy a single orbital?
a) 1
b) 2
c) 3
d) 4

Given that the principal quantum number, n, is 2, write down the allowed values of l and m_l, and determine the number of atomic orbitals possible for $n = 3$.

For a given value of n, the allowed values of l are $0, 1, 2 \ldots (n-1)$, and those of m_l are $-l \ldots 0 \ldots +l$.

For $n = 2$, allowed values of $l = 0$ or 1.

For $l = 0$, the allowed value of $m_l = 0$.

For $l = 1$, allowed values of $m_l = -1, 0, +1$

Each set of three quantum numbers defines a particular atomic orbital, and, therefore, for $n = 2$, there are four atomic orbitals with the sets of quantum numbers:

$$n = 2, \quad l = 0, \quad m_l = 0$$

$$n = 2, \quad l = 1, \quad m_l = -1$$

$$n = 2, \quad l = 1, \quad m_l = 0$$

$$n = 2, \quad l = 1, \quad m_l = +1$$

Using the rules that govern the values of the quantum numbers n and l, write down the possible types of atomic orbital for $n = 1$, 2 and 3.

The allowed values of l are integers between 0 and $(n - 1)$.
For $n = 1$, $l = 0$.
The only atomic orbital for $n = 1$ is the 1*s* orbital.

For $n = 2$, $l = 0$ or 1.
The allowed atomic orbitals for $n = 2$ are the 2*s* and 2*p* orbitals.

For $n = 3$, $l = 0$, 1 or 2.
The allowed atomic orbitals for $n = 3$ are the 3*s*, 3*p* and 3*d* orbitals.

Write down two possible sets of quantum numbers that describe an electron in a 2*s* atomic orbital. What is the physical significance of these unique sets?

The 2*s* atomic orbital is defined by the set of quantum numbers $n = 2$, $l = 0$, $m_l = 0$.

An electron in a 2*s* atomic orbital may have one of two sets of four quantum numbers:

$$n = 2, \quad l = 0, \quad m_l = 0, \quad m_s = +\tfrac{1}{2}$$

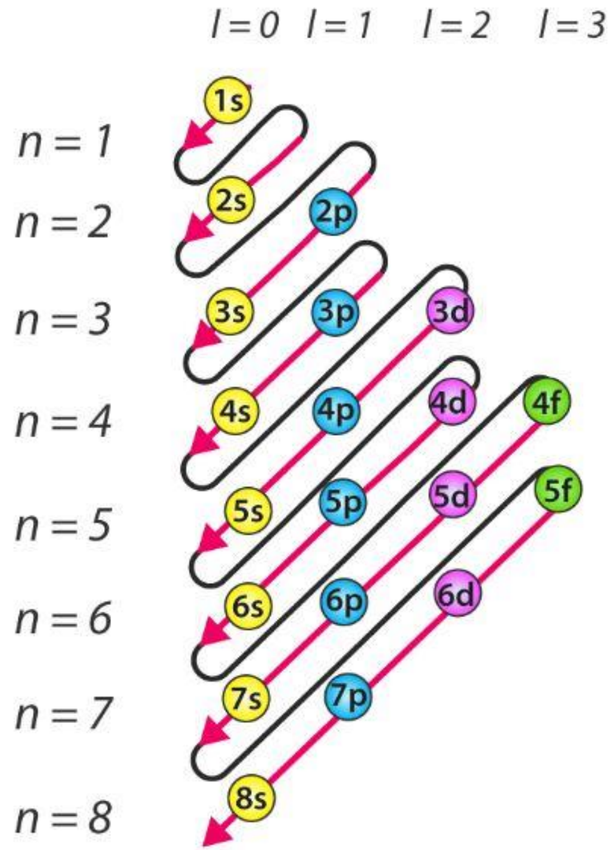
or

$$n = 2, \quad l = 0, \quad m_l = 0, \quad m_s = -\tfrac{1}{2}$$

If the orbital were fully occupied with two electrons, one electron would have $m_s = +\frac{1}{2}$, and the other electron would have $m_s = -\frac{1}{2}$, i.e. the two electrons would be spin-paired.

Aufbau Principle

- The Aufbau principle states that electrons fill atomic orbitals in order of increasing energy.
- Here lower energy orbitals are filled before higher energy orbitals.
- Electrons occupy orbitals in a specific sequence dictated by the increasing order of their principal quantum numbers (n) and azimuthal quantum numbers (l).
- Energy levels are decided based on their (n+l) values. Consider 4s and 3d
- When two orbitals have same (n+l) values, the one with lower n value is filled first.
- The Aufbau principle helps to determine the electron configurations of atoms and their placement in different energy levels and subshells.

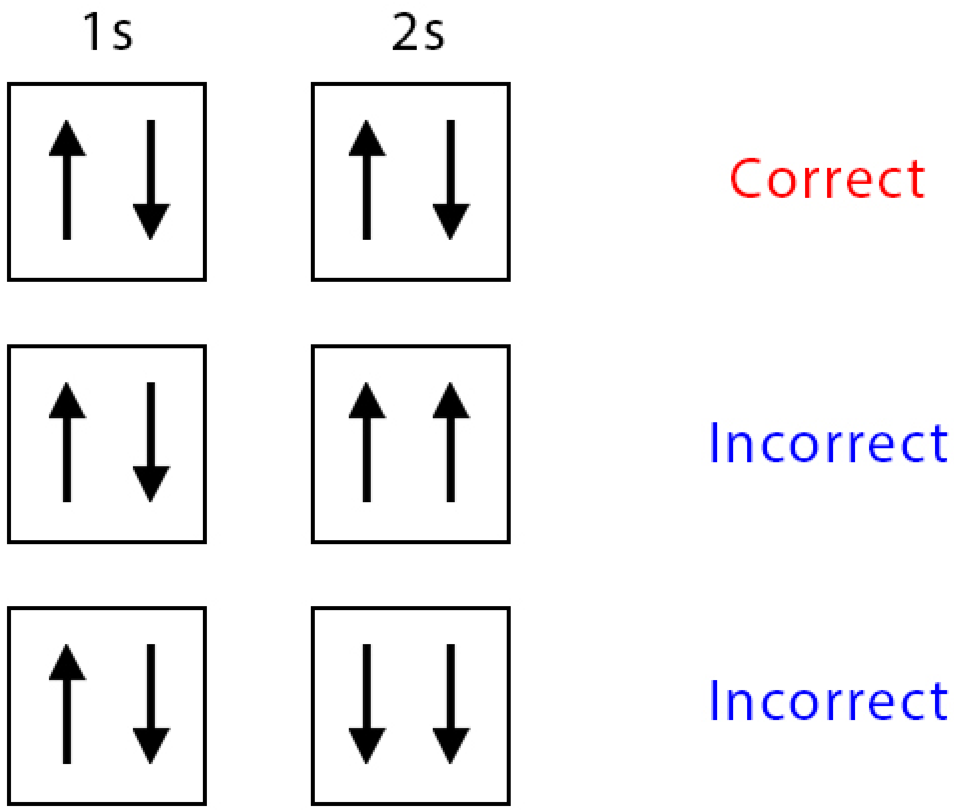


PAULI'S EXCLUSION PRINCIPLE

- Pauli's exclusion principle states that no two electrons within an atom can have the same set of four quantum numbers.
- This principle emphasizes that each electron must have a unique combination of quantum numbers, including the principal quantum number (n), azimuthal quantum number (l), magnetic quantum number (ml), and spin quantum number (ms).
- As a result, only two electrons can occupy a single atomic orbital, and they must have opposite spins (ms values of +1/2 and -1/2).
- Pauli's exclusion principle ensures the stability of electron configurations and determines the nature of chemical bonding and electron interactions.
- On the basis of Pauli's E P, it can be stated that **maximum number of electrons that can be accommodated in an orbital is two**

Pauli Exclusion Principle

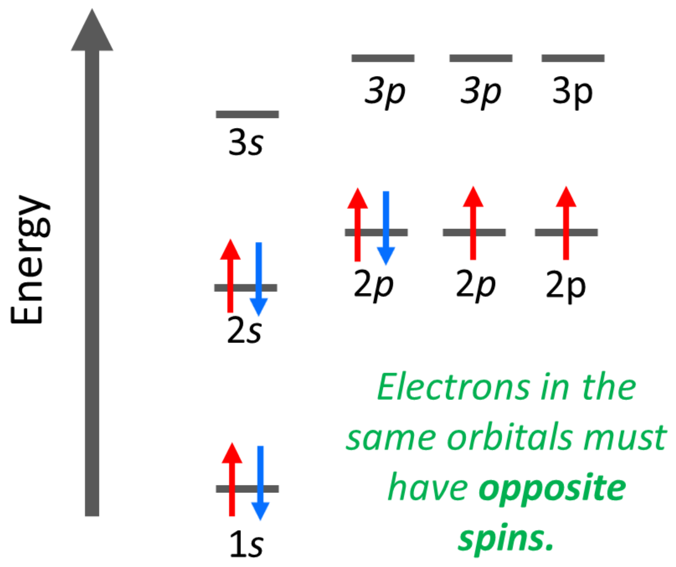
No two electrons can have the same set of quantum numbers



↑ Electron spin up ($m_s = +1/2$) ↓ Electron spin down ($m_s = -1/2$)

Pauli's Exclusion Principle

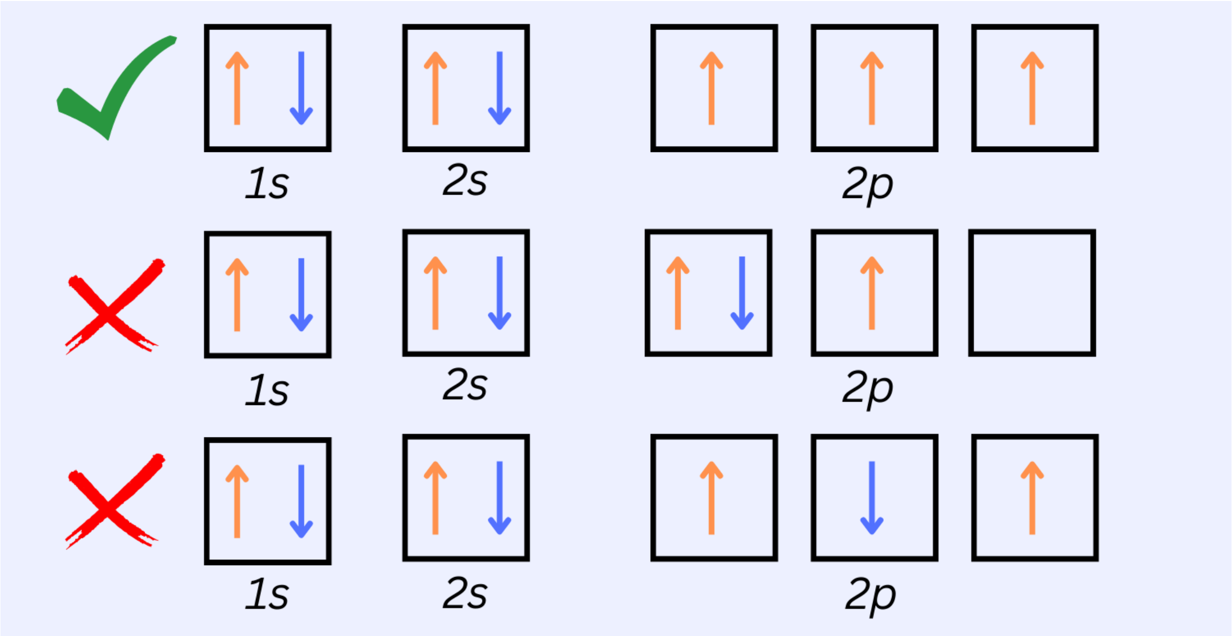
No two electrons in an atom can have the **same *four* quantum numbers.**



This is because when they are in the **same orbital, the values of *n*, *l*, and m_l are the same**. Therefore, they **must have opposite spins (different m_s)** so that they do not have all four quantum numbers the same.

HUND’S RULE

- Hund's rule states that when multiple degenerate orbitals are available at the same energy level, electrons fill these orbitals singly, with parallel spins, before pairing up.



This rule highlights the preference of electrons to occupy different orbitals within the same subshell, maximizing the total electron spin and promoting electron-electron repulsion.

By occupying different orbitals, electrons spread out and experience less electron-electron repulsion, resulting in lower energy configurations.

Hund's rule helps explain the stability and magnetic properties of atoms and ions.

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