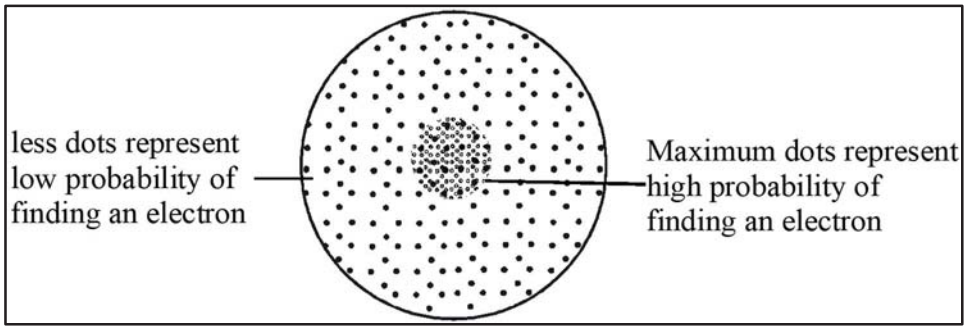
SHAPE OF ATOMIC ORBITALS

Orbital

An orbital can be described as the space around the nucleus where the probability of finding an electron is at its maximum (typically 90% to 95%).

Orbitals do not specify a precise path for the electron; instead, they indicate only the likelihood of the electron being in different regions of space around the nucleus.



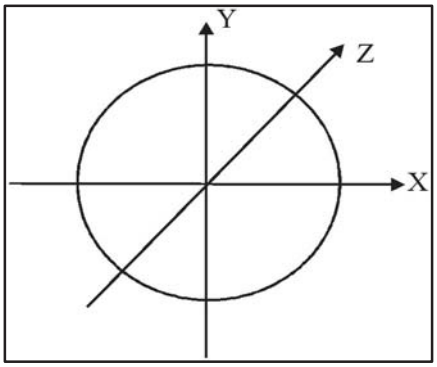
Difference Between Orbit and Orbitals

S.No.	Orbit	Orbitals
1.	It is well defined circular path followed by It is well defined circular path followed by	It is the region of space around the nucleus where electron is most likely to be found
2.	It represents planar motion of electron	It represents 3-dimensional motion of an electron around the nucleus.
3.	The maximum no. of electron in an orbit is $2n^2$ where n stands for no. of orbit.	Orbitals cannot accommodate more than 2 electrons.
4.	Orbits are circular in shape.	Orbitals have different shape e.g., s-orbital is spherical, p - orbital is dumb-bell shaped.
5.	Orbit are non-directional in character. Hence, they cannot explain shape of molecules	Orbitals (except s-orbital) have directional character. Hence, they can account for the shape of molecules.
6.	Concept of well-defined orbit is against Heisenberg's uncertainty principle.	Concept of orbitals is in accordance with Heisenberg's principle

Shape of The Orbitals

The shapes of orbitals are determined by solutions to the Schrödinger wave equation, indicating the space in which the probability of finding an electron is highest.

s- Orbital: Shape spherical



The s-orbital is non-directional and is situated closest to the nucleus, possessing the lowest energy. It can accommodate a maximum of two electrons.

↑	↓
n	s

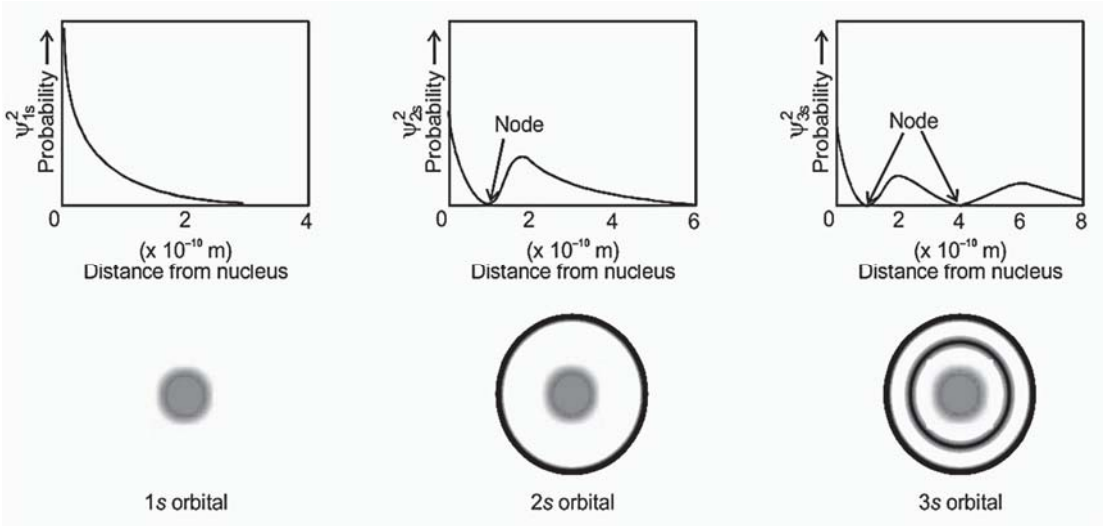
Radial Partiality Distribution

In our exploration of electron behavior within an atom, understanding the probability of locating an electron at a specific distance from the nucleus becomes crucial. This probability is quantified through the Radial Probability Distribution, focusing on the likelihood of finding an electron within an infinitesimally thin spherical shell characterized by a radius, denoted as 'r,' around the nucleus.

For the 1s orbital, the expression $4\pi r^2\Psi^2$ attains its maximum value at $r = 0.529$ Å, providing insights into the region where the electron is most likely to be found.

However, intriguingly, as we extend our analysis to the 2s atomic orbitals, a new feature called a "node" emerges. A node represents a point or region in space where the wave function exhibits zero amplitude, indicating a zero probability of finding the electron at that specific location. The appearance of a node introduces a distinctive aspect to the electron distribution plots, and for 2s orbitals, a single node is observed. Similarly, the 3s orbital displays the presence of two nodes.

Visual representations of electron probability distribution, as well as cutaway density depictions, are provided for 1s, 2s, and 3s orbitals. While all three orbitals exhibit spherical symmetry, the 2s orbital is encapsulated within a spherical surface of zero probability (node), and the 3s orbital is enclosed within two such spherical surfaces of zero probability.



The figure presented illustrates the three-dimensional space around the nucleus where the probability of finding an electron exceeds 95%. This graphical representation serves as a visual depiction of the square of the wave function (Ψ^2).

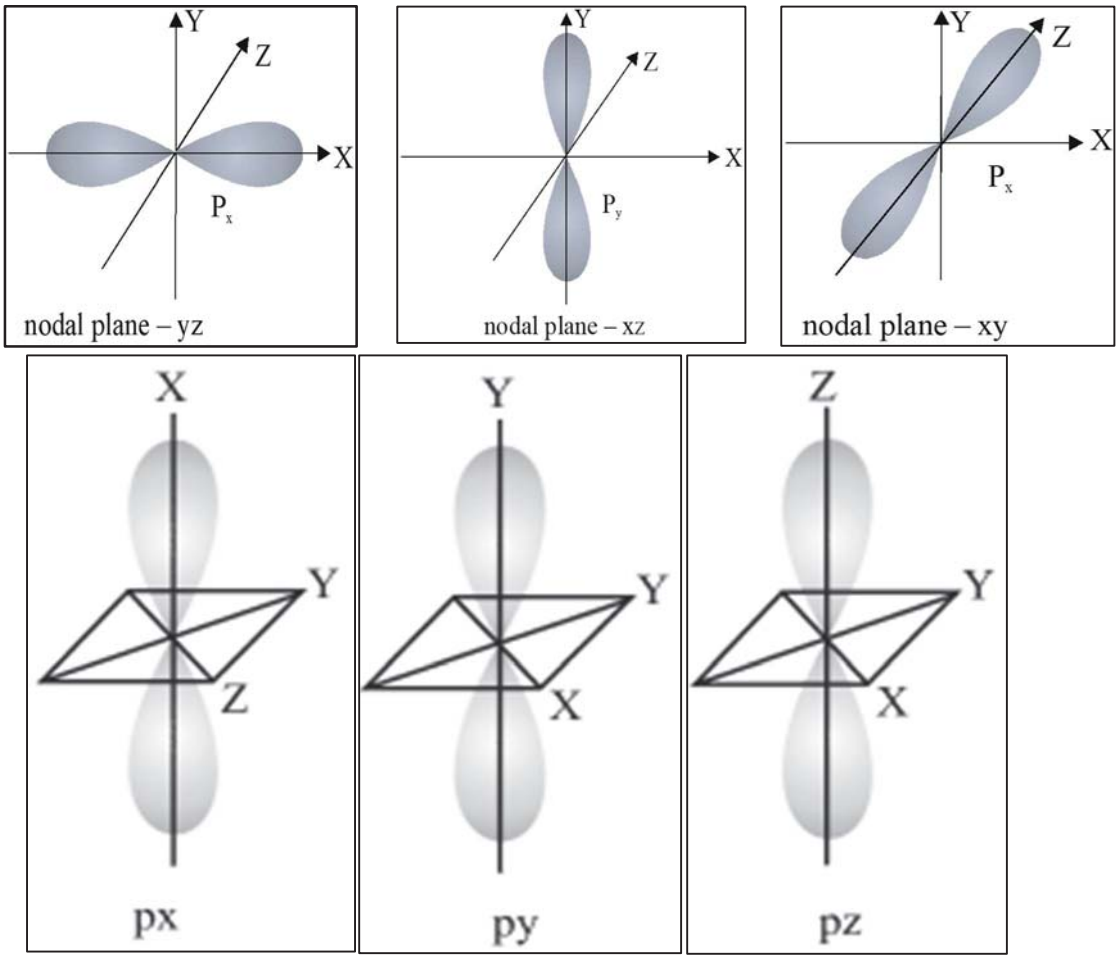
For the s subshell, where the azimuthal quantum number (l) is 0, and the magnetic quantum number (m) is also 0, only one type of orbital is present within this subshell. This characteristic further contributes to the unique features and properties associated with s subshells in atomic orbitals.

p-Orbital

The dumbbell shape is characterized by two lobes separated by a region of zero probability known as a node.

Nodal Plane

The imaginary plane where probability of finding an electron is zero.

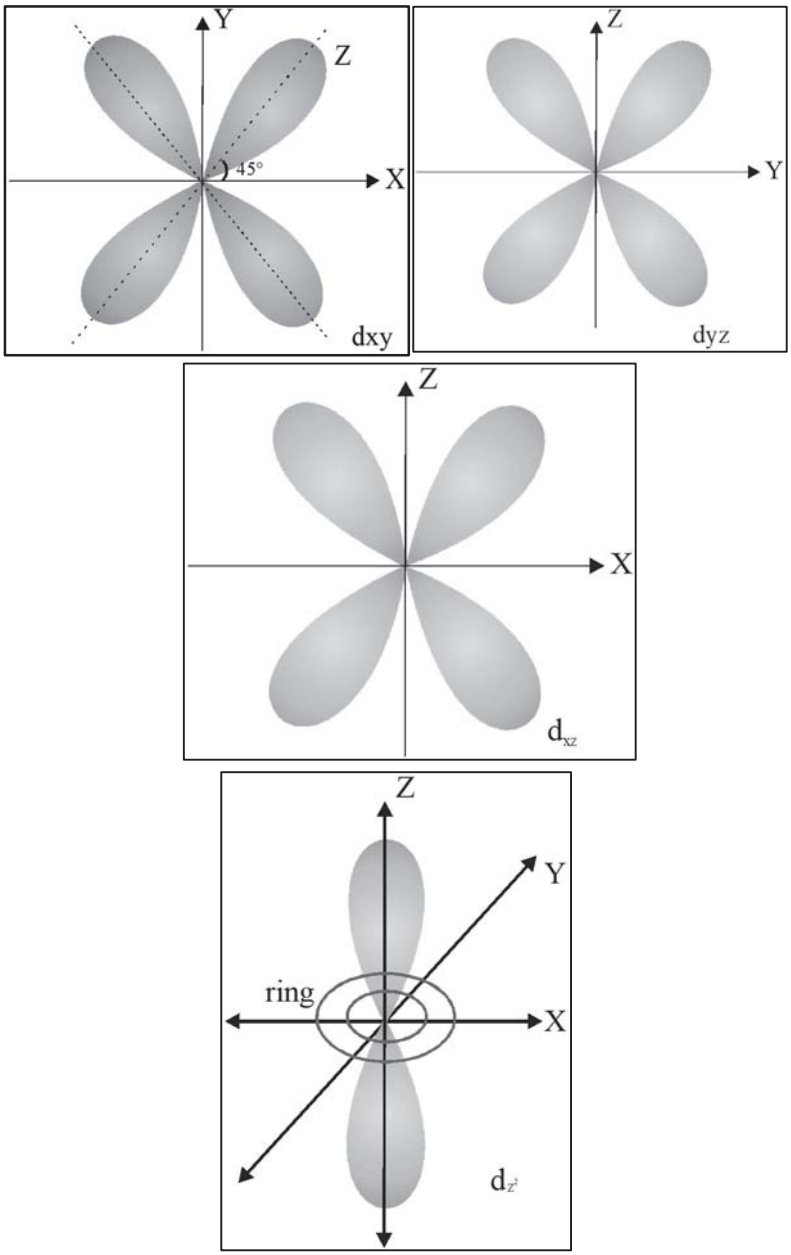


p - subshell can accomodate maximum of six electrons.

↑↓	↑↓	↑↓
P_x	P_v	P_x

d - Orbital

Shape double dumb bell



d - subshell can accomodate maximum of 10 electrons.

↑↓	↑↓	↑↓	↑↓	↑↓
dxy	dyz	Dz^2	$Dx^2 – y^2$	dxz

f - Orbital

Shape leaf like or Complex

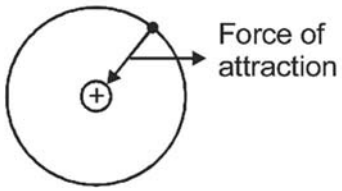
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓

f - orbital can accomodate maximum no. of 14 electrons.

Energies of Atomic Orbitals

Single-Electron Interaction

The rationale underpinning this energy sequence stems from the unique circumstance of a hydrogen atom harboring only one electron. Consequently, the singular electrical interaction present is the attractive force between the negatively charged electron and the positively charged nucleus.



Degenerate Orbitals

Degenerate orbitals refer to orbitals sharing identical energy levels. In the presented case, 3s, 3p, and 3d orbitals exhibit this phenomenon.

Ground State

The ground state denotes the electron's most stable configuration. In this state, the electron resides in the orbital with the minimum energy, tightly bound by the attractive force exerted by the nucleus. Hence, the 1s orbital in a hydrogen atom is recognized as the ground state.

Excited State

An electron occupying higher energy orbitals, such as 2s, 2p, or beyond, is described as being in an excited state. This state signifies an increased energy level beyond the ground state, illustrating the dynamic behavior of electrons within the hydrogen atom.

Shielding Effect

The Shielding Effect (σ) refers to the protective influence exerted by inner-shell electrons, mitigating the nuclear force experienced by outer-shell electrons in an atom. As a consequence of this shielding, the actual nuclear charge perceived by the outer-shell electrons is termed the effective nuclear charge (Z_{eff}), and it is calculated as the difference between the actual nuclear charge (Z) and the shielding effect (σ).

$$Z_{eff} = Z - \sigma$$

Despite the shielding, the attractive force acting on outer-shell electrons intensifies with an augmentation in nuclear charge. It is crucial to note that a stronger attractive force corresponds to a decrease in energy (i.e., a more negative value).

The magnitude of the shielding effect relies on the nature of the orbital housing the inner-shell electrons. The sequence of shielding effect for orbitals is as follows:

$$S > p > d > f$$

In this hierarchy, s-orbital electrons exhibit the most effective shielding of outer-shell electrons from the nucleus. The shielding effect diminishes in p-orbitals but remains more substantial than that of electrons in d-orbitals. Furthermore, the f-orbital electrons provide less shielding to outer-shell electrons compared to d-orbitals. This sequence holds true when all orbitals are situated within the same energy shell.

Consequently, it can be asserted that with an increase in the azimuthal quantum number, the shielding effect diminishes. Consequently, the effective nuclear charge experienced by outer electrons undergoes an increase, emphasizing the intricate interplay between electron distribution and nuclear forces within an atom.