Orbitals

The region around a nucleus in which an electron has a probability of being located is called an orbital.

Orbitals vary in:

- Distance from the nucleus (radial function)
- Direction (angular function)
- Energy

Wavefunction Ψ - mathematical function that describes the wave-like nature of an electron $\Psi(r, \theta, \phi)$

Schrodinger equation - $H\Psi = E\Psi$

Ψ^2 - probability distribution map of the electron

Quantum Numbers

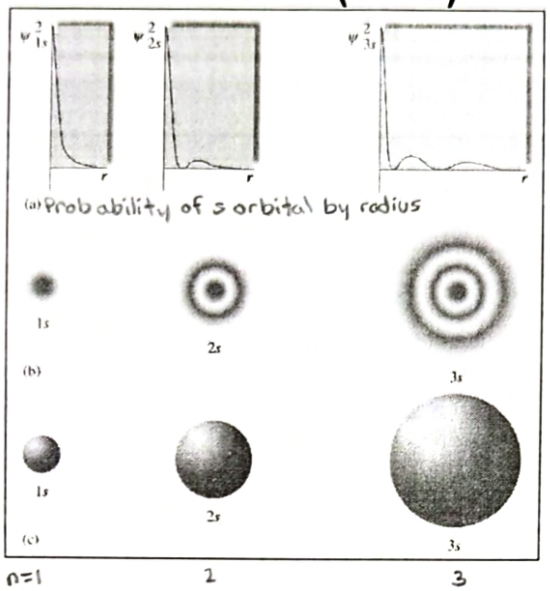
Each orbital is characterized by a set of quantum numbers.

Principal Quantum number (n) - shell
Allowed values: 1, 2, 3, ...
Related to size and energy of orbital

Angular Quantum Number (ℓ) - subshell
Allowed values: 0 to n-1
Related to orbital shape

$\ell = 0 \rightarrow$ s orbital
$1 \rightarrow$ p orbital
$2 \rightarrow$ d orbital
$3 \rightarrow$ f orbital
$4 \rightarrow$ g orbital

s Orbitals (l = 0)



Quantum Numbers (Continued)

Magnetic Quantum Number (m_ℓ)

Indicates the number of orbitals in a subshell with a given quantum number

Allowed values: $-\ell$ to ℓ

$n = 2$

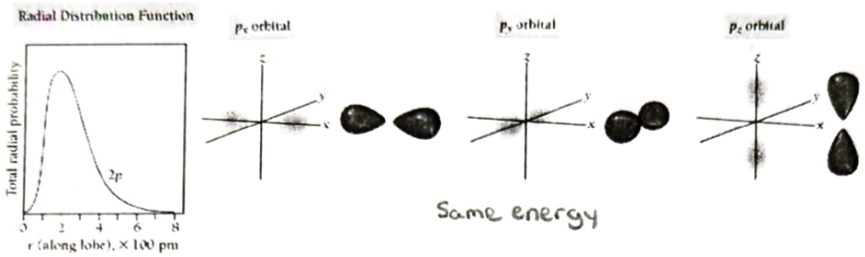
$\ell = 1$ $\quad 2p_x, 2p_y, 2p_z$

$m_\ell = -1, 0, 1$

Equal energy (degenerate)

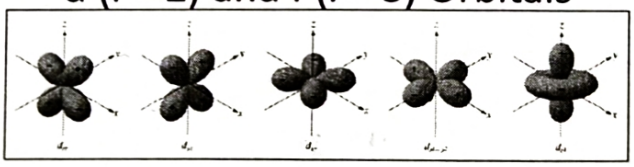
Specifies orientation of orbitals in space

p Orbitals (l = 1)

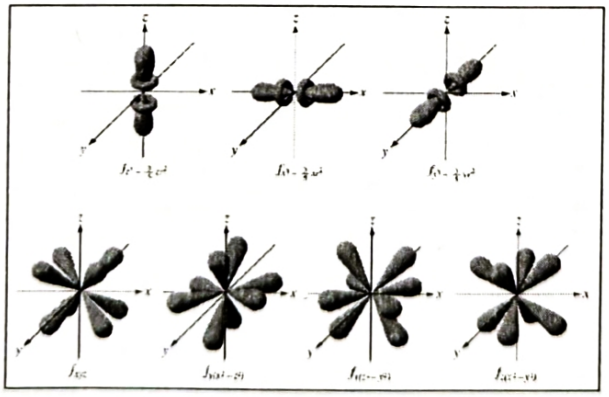


Same energy

d (l = 2) and f (l = 3) Orbitals



m = 3
ℓ = 0, 1, 2
m_ℓ = -2, -1, 0, 1, 2
5 d orbitals



m = 4
ℓ = 0, 1, 2, 3
m_ℓ = -3, -2, -1, 0, 1, 2, 3
7 f orbitals

Quantum Numbers (Continued)

Electron Spin Quantum Number (m_s)

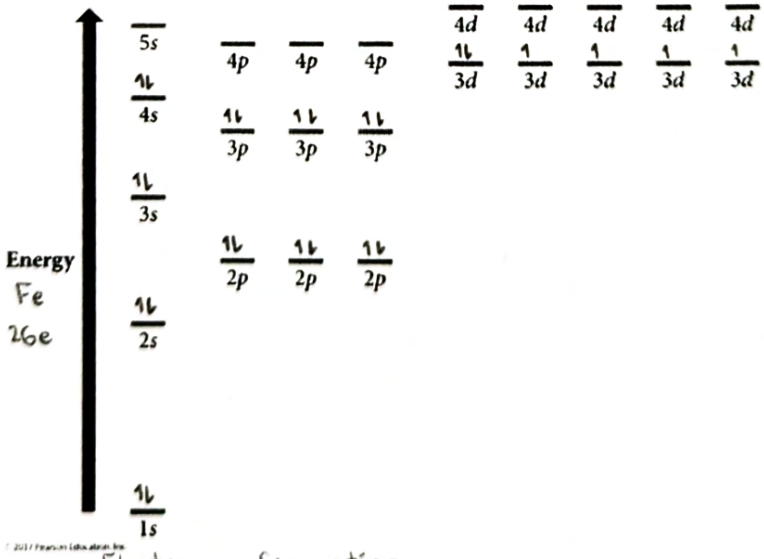
Spin up or spin down

Allowed values: $-\frac{1}{2}$ (↓), $\frac{1}{2}$ (↑)

Pauli exclusion principle: In a given atom no two electrons can have the same four quantum numbers.

An orbital can only hold 2 electrons, and they must have opposite spin.

General Energy Ordering of Orbitals for Multielectron Atoms



Electron configuration

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$