

General Chemistry

Atomic Structure

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by Aini Norhidayah

<http://ocw.ump.edu.my/course/view.php?id=479>

Chapter Description

- Expected Outcome:

At the end of the lecture, the students should be able to understand and solve the problems regarding Atomic model, Quantum mechanical model and electron configuration.

- Reference:

- 1) Martin S. Silberberg. Principles of General Chemistry. McGraw-Hill.
- 2) Raymond Chang. General Chemistry: The essential concepts. McGraw-Hill.



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Contents

- Bohr's Atomic Model
- Electronic configuration
- Quantum Mechanical Model



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Bohr's Atomic Model

Bohr's Postulates:

- An electron moves in a circular path (orbit) around the nucleus of an atom, but the electron does not radiate or absorbing any energy
- Energy of an electron is quantised



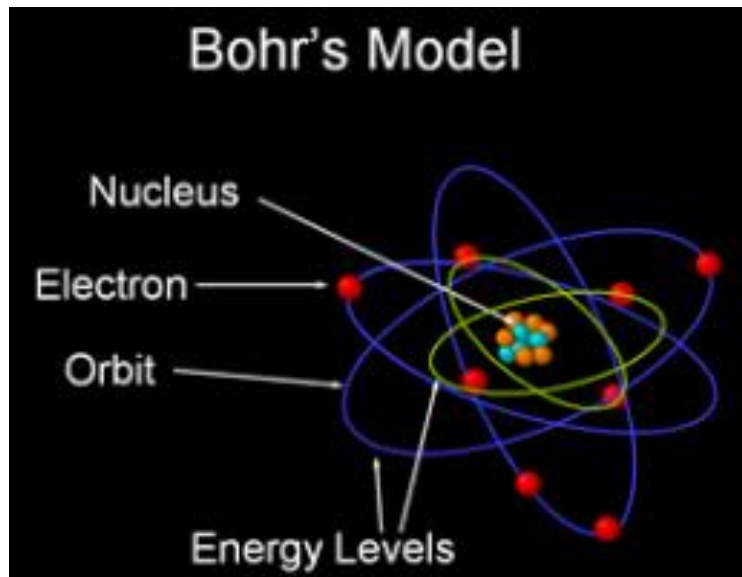
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Bohr's Atomic Model

- Picture source:

<http://byjus.com/chemistry/bohrrs-atomic-model-and-its-limitations/>

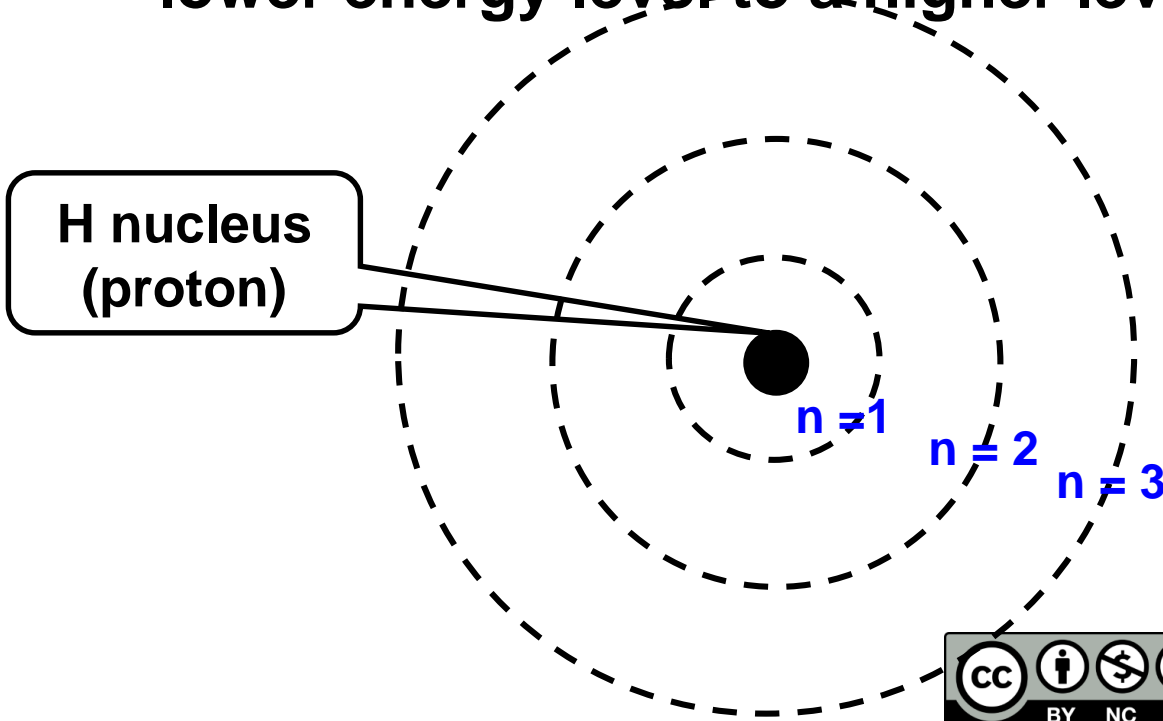


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Bohr's Postulate

- At ordinary condition the electron is at the ground state (lowest level). If energy is supplied, electron will absorb the energy and promoted from lower energy level to a higher level



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Bohr's Postulate

Electron at excited states is unstable. It will go back to lower energy level and releases energy in form of light.



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ENERGY DIFFERENCE during transition (ΔE)

$$E_{\text{photon}} = \Delta E = E_f - E_i$$

$$E_f = -R_H \left(\frac{1}{n_f^2} \right) \qquad E_i = -R_H \left(\frac{1}{n_i^2} \right)$$

Energy differences between two levels:

$$\begin{aligned} \Delta E &= R_H \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \\ &= h\nu \end{aligned}$$

Note: i = initial ; f = final



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- The amount of energy released is called a photon
- Photon is emitted in the form of radiation with a frequency and wavelength.

$$\Delta E = h\nu$$

$$\nu = \frac{c}{\lambda}$$

$$\Delta E = \frac{hc}{\lambda}$$

λ : wavelength (m)

c : speed of light = 3.00×10^8 m/s

h : planck constant = 6.63×10^{-34} Js



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Electron configuration

**Shows how electrons are distributed
in various atomic orbitals**

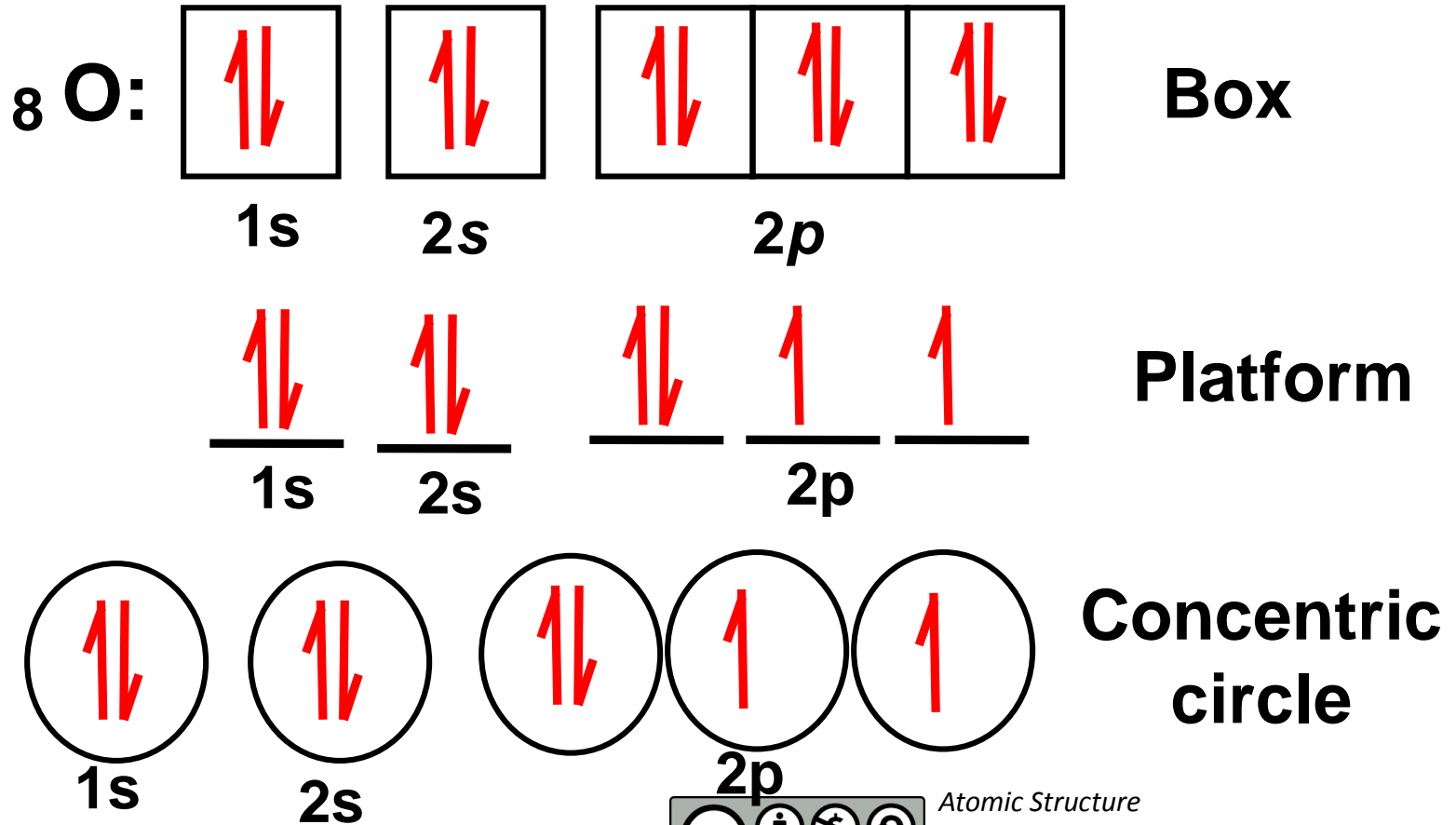


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Representing electronic configuration

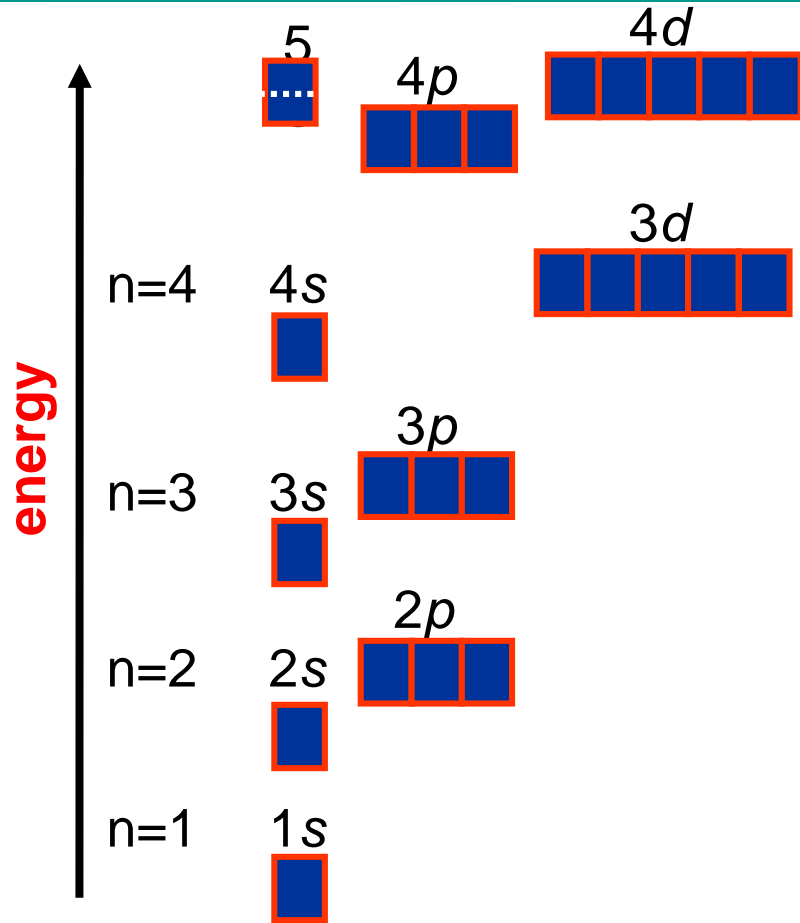
- Method 1: Orbital diagram



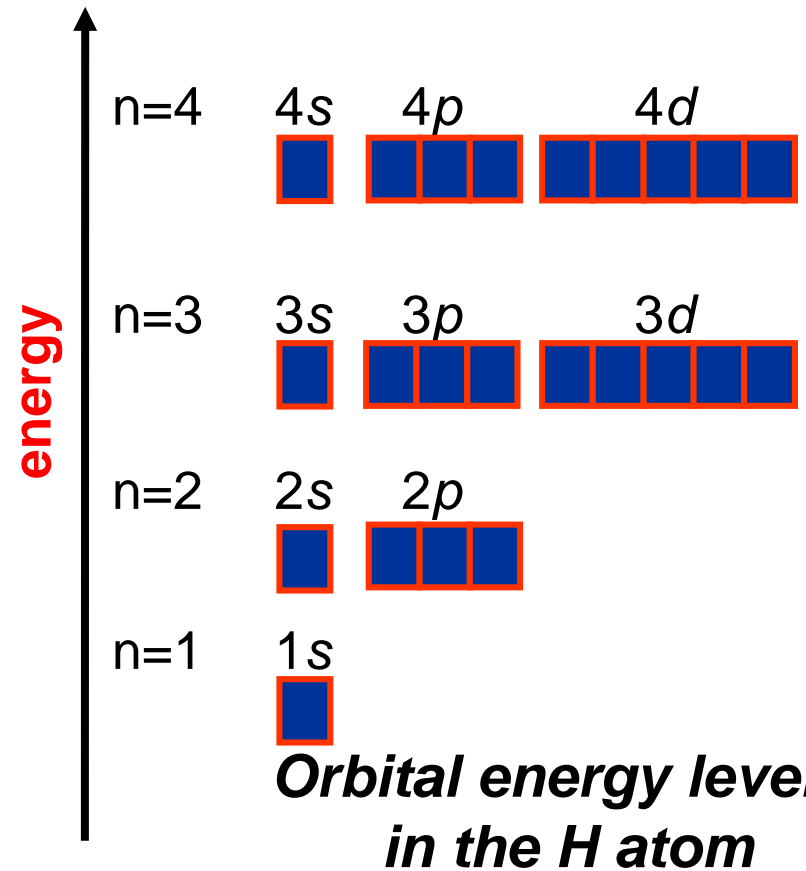
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Relative energy of atomic orbital



**Orbital energy levels
in a many-electron atom**



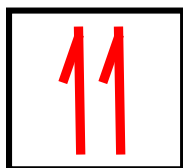
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Pauli Exclusion Principle

No 2 electrons in the same atom can have same quantum numbers

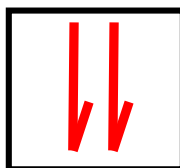
He atom
 $1s^2$



$(1,0,0, +\frac{1}{2})$

$(1,0,0, +\frac{1}{2})$

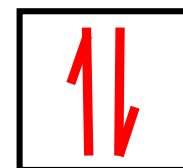
**WRONG
WAY**



$(1,0,0, -\frac{1}{2})$

$(1,0,0, -\frac{1}{2})$

**WRONG
WAY**



$(1,0,0, +\frac{1}{2})$

$(1,0,0, -\frac{1}{2})$

correct



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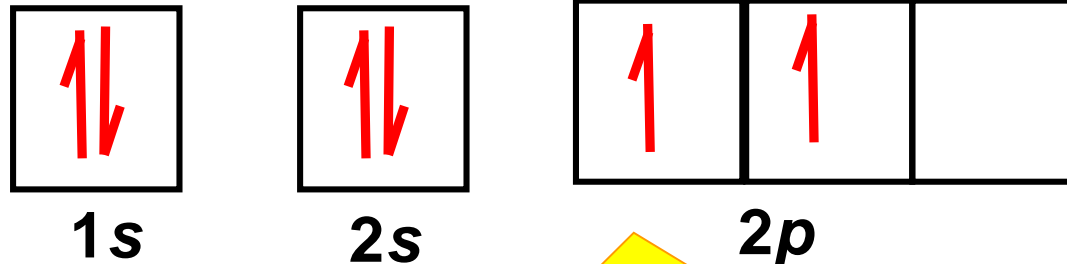
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Hund's Rule

Before any one orbital is doubly occupied, every orbital in a subshell is singly occupied with one electron

All electrons in singly occupied orbitals have the same spin.

C (Z = 6)



**number of parallel
spin = 2**



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Quantum number

Principal quantum number (n)

Angular momentum quantum number (ℓ)

Magnetic quantum number (m)

electron spin quantum number (s)




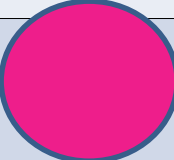
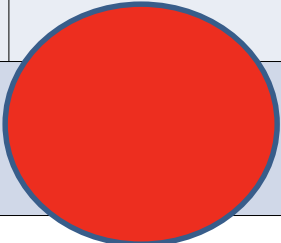


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Principle of Quantum number

The *value of n* determines the *energy* of an orbital thus determining the energy of an electron in that particular orbital

n	1	2	3	4
shell	K	L	M	N
Orbital size	increase 			
Energy				



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Angular momentum number

ℓ = Integer 0 to $(n - 1)$

Indicates the shape and types of orbital

n determine ℓ

EXAMPLE:

$$n = 1 \quad \ell = 0$$

$$n = 2 \quad \ell = 0, 1$$

$$n = 3 \quad \ell = 0, 1, 2$$



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Magnetic quantum number

$m =$ integer from $-\ell$ through 0 to $+\ell$

Indicates orientation of orbital in the space around the nucleus

ℓ determine m

Number of possible m values = $2\ell + 1$

EXAMPLE:

1 possible orbitals
(s subshell)

3 possible orbitals
(p subshell)

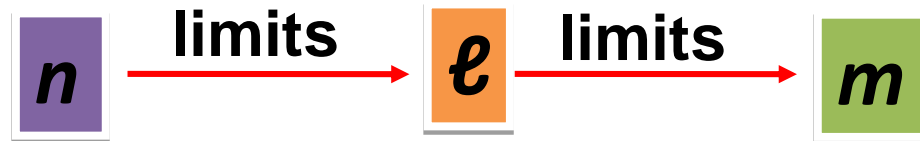
$$\ell = 0 \quad m = 0$$

$$\ell = 1 \quad m = -1, 0, +1$$

$$\ell = 2 \quad m = -2, -1, 0, +1, +2$$

5 possible orbitals
(d subshell)

Hierarchical relationship



EXAMPLE:

$n = 2$ possible l values = 0 , 1

$l = 1$ possible m values = - 1 , 0 , +1

$l = 0$ possible m values = 0

■ max no. of $e^- = 2n^2$



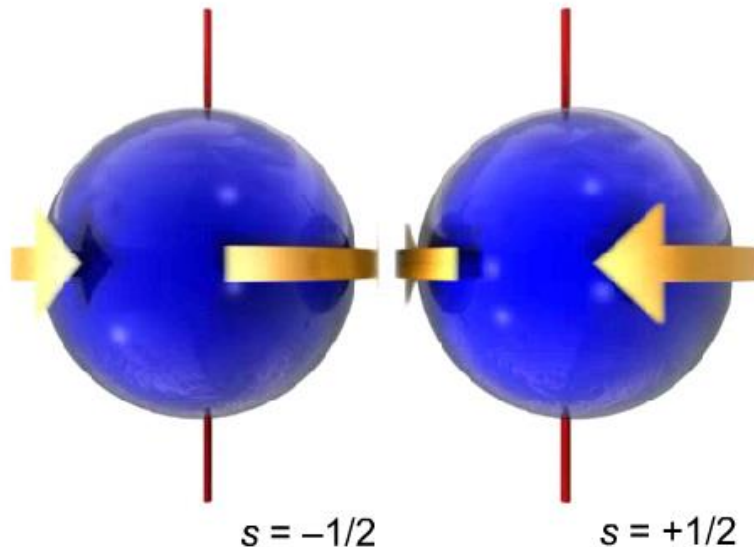
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Electron Spin Quantum Number

s value of : $+1/2$ and $-1/2$

Two possible motions of an electron
☞ **clockwise and anti-clockwise**



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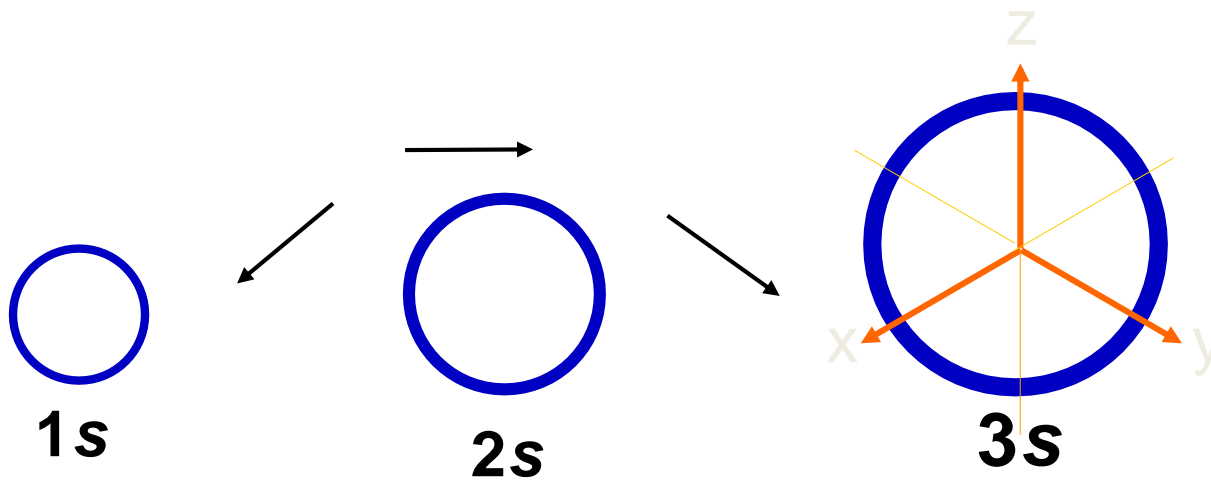
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Shape of s orbital

Spherical shape with nucleus at the center

2s orbital larger than 1s

Only have 1 orientation ($\ell = 0, m = 0$)



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Shape of p orbital

- When $\ell = 1$
- Dumbbell shaped
- 3 p -orbitals p_x , p_y , and p_z .
- Correspond m of -1, 0, and +1.
- As n increases, the p -orbitals get larger.
- All p -orbitals have a node at the nucleus.



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Shape of d orbital

- 4 d orbitals have 4 lobes (perpendicular),
- 1 d orbital has 2 major lobes along z axis and a donut-shaped girdles the center.

When $\ell = 2$

$m = -2, -1, 0, 1, 2$

the orbitals are: d_{yz} , d_{xz} , d_{xy} , $d_{x^2-y^2}$, d_{z^2}



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Author Information

Aini Hidayah Mohamed is a lecturer from Faculty of Industrial Sciences & Technology Industry, Universiti Malaysia Pahang, Malaysia. She is also a chemist who has experiences in general chemistry, industrial chemistry and natural product subject.



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