Announcements (Week 2- Sept 11th to 15th)

Quiz 1 is open and due on Friday – all details posted on myCourses. 1 attempt; 5 questions. The quiz will cover Concept Videos 1, 2, and 3 (i.e. last week's content)

Office Hours with Prof. Sirjoosingh:

Thursday 3 to 4:30 PM (Location TBA)

Peer Collab with TAs/TEAM Mentors:

Monday and Wednesday 3 to 5 pm (2001 McGill College Avenue)

For any questions related to the course – please email chem110-120.chemistry@mcgill.ca

Optical Smoke Detectors

Chemistry around us!

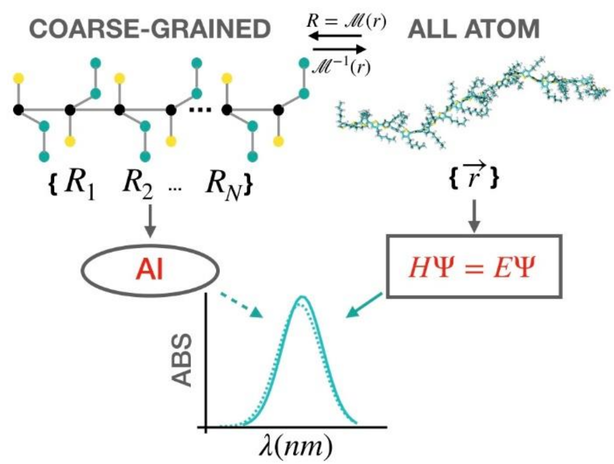
- Use the principles of photoelectric effect
- Contains source of light, a lens and a photoelectric receiver.

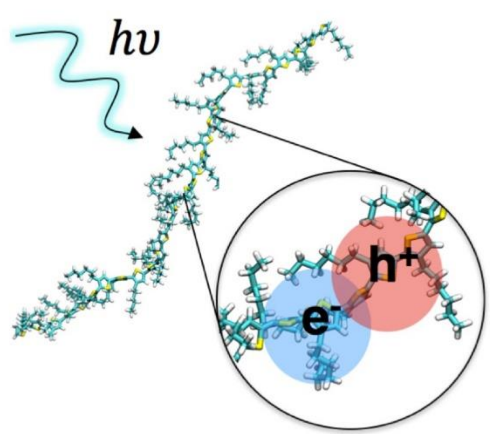
In some optical smoke detectors: light being produced by a light source, detected by the photosensor.

tps://www.siminegroup.ca/researchers

In the presence of smoke, the light intensity being detected is reduced (scattering due to smoke) generating an alarm, if the intensity is below a certain threshold.

Lena Simine (Department of Chemistry)



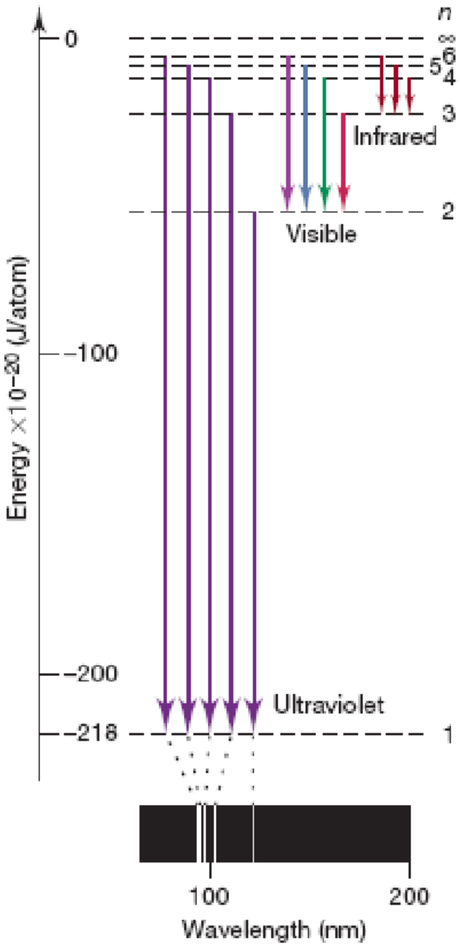


This is what a Chemist looks like

- Computational chemist at McGill
- Development of computational models to describe behavior of molecules at atomic level
- Adaptation/development of machine learning to understand and predict properties of materials
- Research on development of organic polymers

https://www.siminegroup.ca/research

Bohr's Model



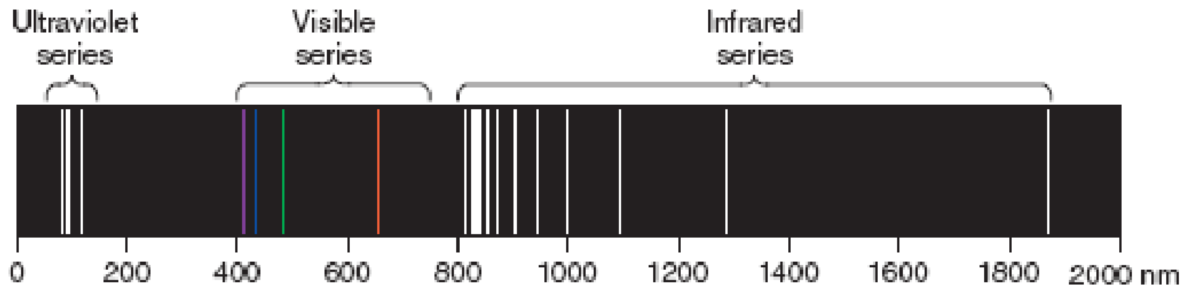
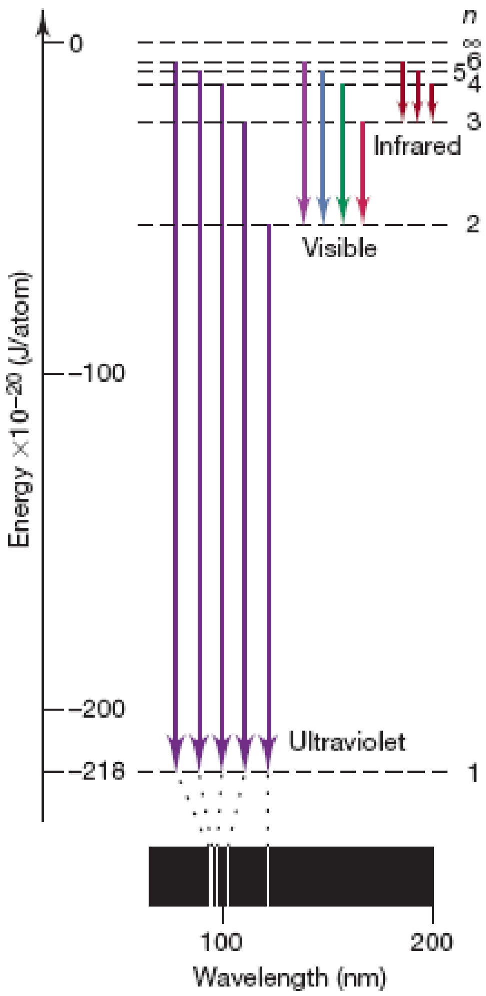


Figure 6.10
Chemistry: The Molecular Nature of Matter and Change
Silberberg, 2e

Bohr's model explains the data for 1-electron species well

Practice Problem 1 (Atomic Spectra)

Calculate the energy required to completely remove an electron (ionize the atom) from the ground state (n =1) of a hydrogen atom?



Practice Problem 1 (Atomic Spectra)

Calculate the energy required to completely remove an electron from the ground state (n =1) of a hydrogen atom and ionize it?

What do we know?

$$E = -2.18 \times 10^{-18}\left(\frac{Z^2}{n^2}\right)$$

Z =1; for H-atom (Atomic Number)

n_{final} is ∞ The electron has been completely removed from the atom; so the orbit number is an infinitely large number

$n_{initial}$ is 1 Ground state that electron is in the lowest energy level – most stable

Calculate E_{final}

$$E_{final} = -2.18 \times 10^{-18}\left(\frac{1^2}{\infty^{\,2}}\right)$$

$E_{final} = 0$ J

Calculate $E_{initial}$

$$E_{initial} = -2.18 \times 10^{-18}\left(\frac{1^2}{1^{\,2}}\right)$$

$E_{initial} = -2.18 \times 10^{-18}$ J

Calculate ΔE for 1 H atom

$$\Delta E = E_{final} - E_{initial} = 0 - \left(-2.18 \times 10^{-18}\right) = 2.18 \times 10^{-18} \text{ J}$$

Practice Problem 2

In the 2007 US Open, Venus Williams hit a serve at 207 km/hr. Calculate the deBroglie wavelength of the tennis ball if it weighed 57.0 g? <u>(3 significant figures)</u>

Practice Problem 2

In the 2007 US Open, Venus Williams hit a serve at 207 km/hr. Calculate the deBroglie wavelength of the tennis ball if it weighed 57.0 g? (3 significant figures)

$h = 6.626 \times 10^{-34}$ Js $= 6.626 \times 10^{-34}$ $kgm^2s^{-2}s$

$\lambda = h/(mu)$

m = 57.0 g – convert to kg = 57.0×10^{-3} kg

$$\lambda = \frac{6.626 \times 10^{-34}\ kgm^2s^{-2}s}{(57.0 \times 10^{-3}\ kg) \times (57.5\ ms^{-1})}$$

u = 207 km/hr – convert to ms^{-1}

= (207 km/hr) x (1000 m/km) x (1 hr/ 3600 s)

= 57.5 m/s

$\lambda = 2.02 \times 10^{-34}$ m

Practice Problem 3

An electron is moving near an atomic nucleus has a speed of 3×10^6 m/s ± 1%. What is the **minimum** uncertainty in its position (Δx)?

Practice Problem 2

An electron is moving near an atomic nucleus has a speed of 3×10^6 m/s ± 1%. What is the **minimum** uncertainty in its position (Δx)?

Equation:
$(\Delta x) \times (\Delta p) \geq h/4\pi$
$\Delta p = m\,\Delta u$
$(\Delta x) \times (m\Delta u) \geq h/4\pi$

$m_e = 9.109 \times 10^{-31}$ kg

$h = 6.62606876 \times 10^{-34}$ J•s

1. Calculate the uncertainty in speed:
$\Delta u = 1\%$ of $u = 0.01\,(3 \times 10^6)$ m/s $= 3 \times 10^4$ m/s

2. Calculate the uncertainty in position:

$\Delta x \geq 2 \times 10^{-9}$ m

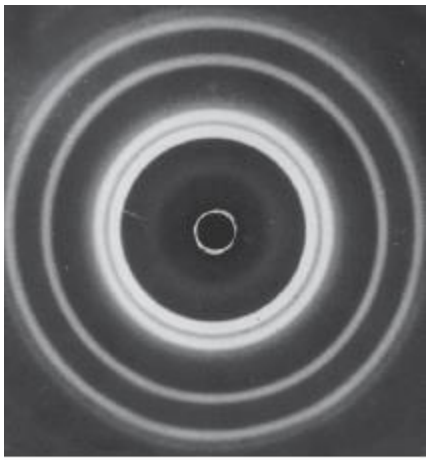
$\Delta x \times m\Delta u \geq h/4\pi$

$$\Delta x \geq h/4\pi(m\Delta u) = \frac{6.626 \times 10^{-34}\ \text{J s}}{(4 \times \pi) \times (9.109 \times 10^{-31}\ \text{kg}) \times (3 \times 10^{4}\ \text{ms}^{-1})}$$

Experiments show that matter has wave-like nature!.....

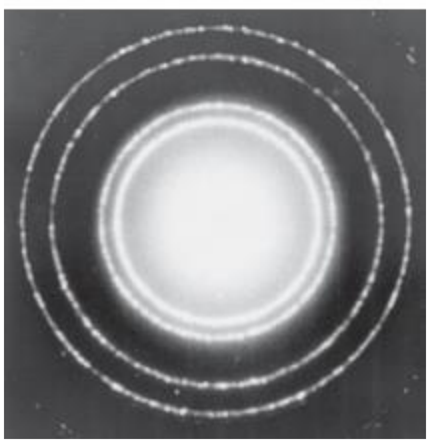
de Broglie's hypothesis was confirmed by experiments by Davisson and Germer

Electrons indeed had wave-like properties



Diffraction pattern of aluminum using X Rays

Light with wave-like properties



Diffraction pattern of aluminum using electrons

Electrons (which make up all matter) with wave-like properties

Quantum Mechanics

Atom can be described in terms of specific quantities of energy depending upon the allowed frequencies of its electrons' wave-like function

Described electron distribution as a *standing wave* and provided solutions for it

Erwin Schrödinger
1887-1961

Schrödinger Equation

$$\hat{H}\psi = E\psi$$

$\hat{H}$: Hamiltonian Operator
E: Binding Energy
Ψ: Wave Function

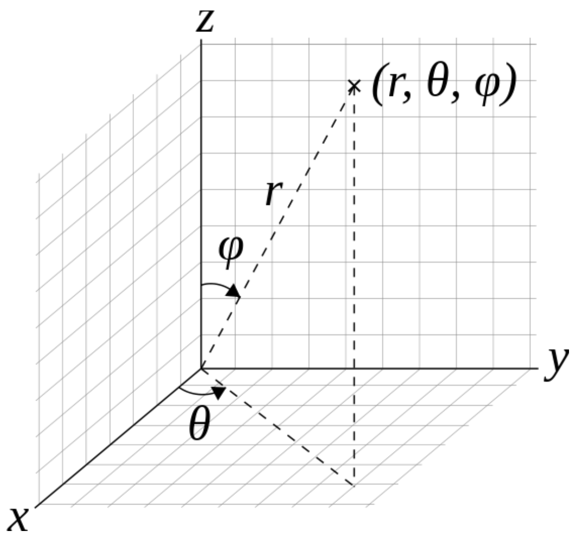
Wave Function (Ψ; pronounced "sai")

A mathematical function that relates the location of an electron at a given point in space to its energy

Wavefunctions

A mathematical function that relates the location of an electron at a given point in space to its energy.

Contains a radial (r) and angular component (θ, φ)



$$\Psi_{n,\,l,\,m}\,(r,\theta,\varphi) = R(r) \times Y_{l,\,m}\,(\theta,\varphi)$$

Each wavefunction is defined by characteristic **quantum numbers** (n, l, m)

The square of the wave function Ψ^2 lets us calculate the **probability of finding an electron** at a given point

Orbitals : Mathematically derived regions of space with different *probabilities* of containing an electron.

Quantum Mechanics

QUANTUM NUMBERS (describing orbitals)

1. Principal Quantum Number (n)

1. Positive integer (1,2,3....)
2. Indicates the relative size of the orbital – relative distance
3. Specifies the energy level (higher n indicated higher energy)

2. Angular Quantum Number (*l*)

1. Positive Integer (0 to n-1)
2. Shape of the orbital
3. The value of n limits *l*

if n=1, *l* can only have the value 0; if n=2, *l* can have the values 0 and 1

When l =0 (s orbital); l=1 (p orbital); l=2 (d orbital); l=3 (f orbital)

3. Magnetic Quantum Number (m_l)

1. Integer (-*l* to +*l*)
2. Orientation of the orbital around the nucleus
3. The value of l limits m_l; For l=1, values of m_l can be -1,0, and 1

Probability Density and Radial Probability (1s orbital)

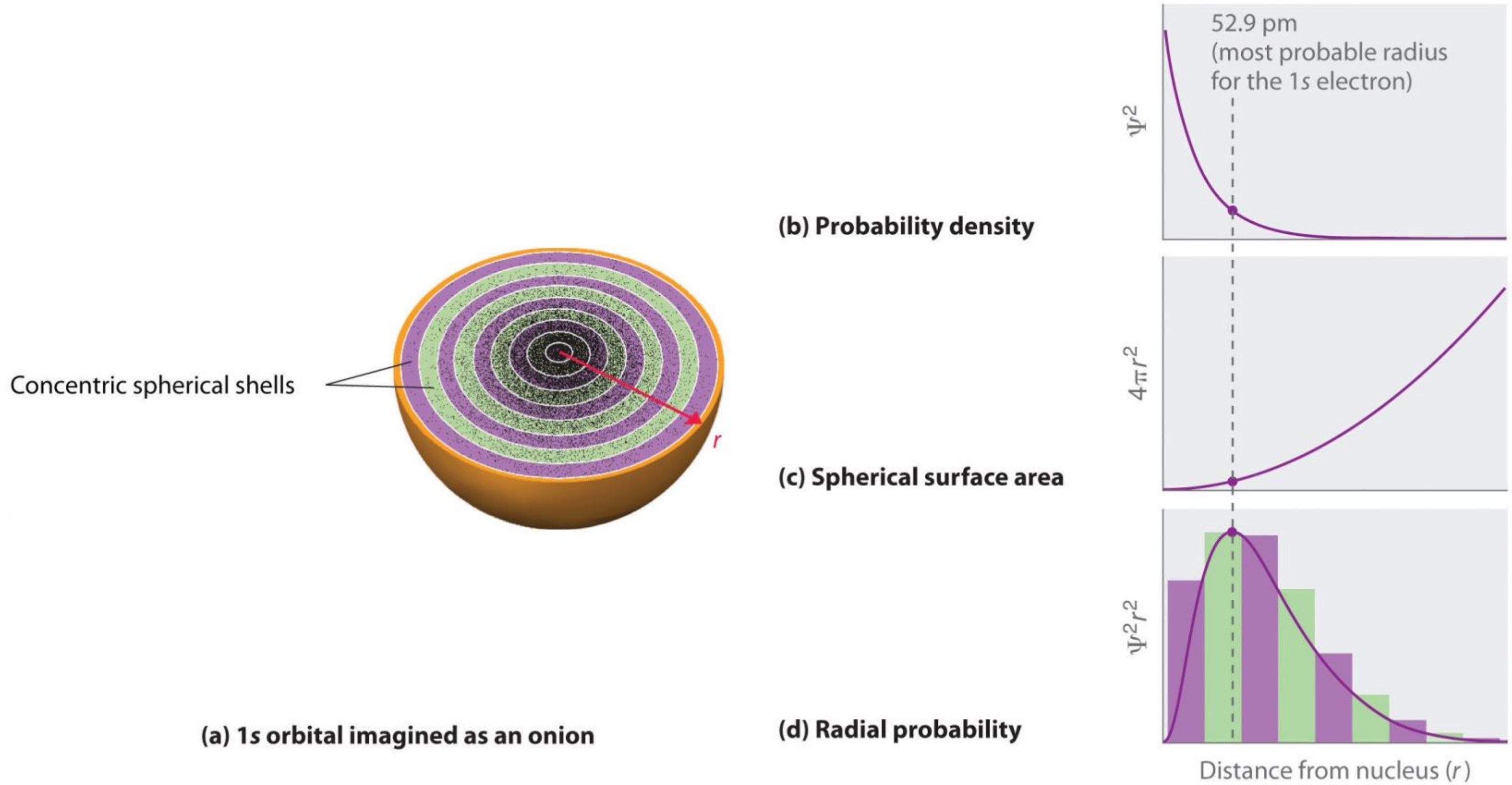


IMAGE COURTESY: [UCDAVIS CHEMWIKI](), [CC BY-NC-SA 3.0 US]()

The probability density can be multiple by volume to obtain the probability of finding an electron at a certain distance from the nucleus

Quantum Mechanics

Erwin Schrödinger
1887-1961

Atom can be described in terms of specific quantities of energy depending upon the allowed frequencies of its electrons' wave-like function

Described electron distribution as a *standing wave* and provided solutions for it

Schrödinger Equation

$$\hat{H}\psi = E\psi$$

$\hat{H}$: Hamiltonian Operator
E: Binding Energy
Ψ: Wave Function

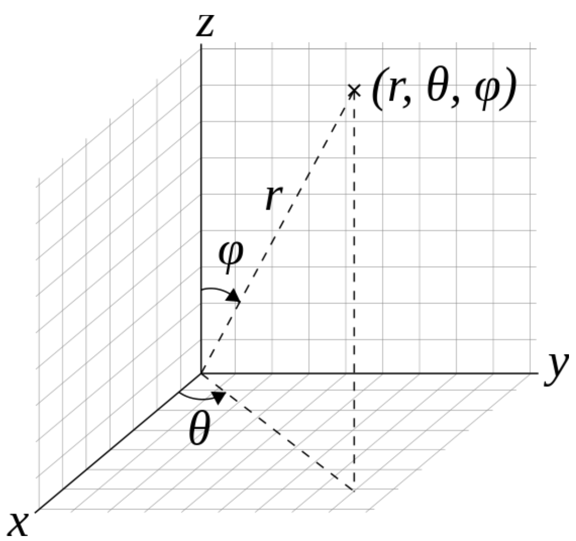
Wave Function (Ψ; pronounced "sai")

A mathematical function that relates the location of an electron at a given point in space to its energy

Wavefunctions

A mathematical function that relates the location of an electron at a given point in space to its energy.

Contains a radial (r) and angular component (θ, φ)



$$\Psi_{n,\, l,\, m}\,(r,\, \theta,\, \varphi) = R(r) \times Y_{l,\, m}\,(\theta,\, \varphi)$$

Each wavefunction is defined by characteristic **quantum numbers** (n, l, m)

The square of the wave function Ψ^2 lets us calculate the **probability of finding an electron** at a given point

Orbitals : Mathematically derived regions of space with different *probabilities* of containing an electron.

Shapes of Atomic Orbital (1s, 2s, 3s orbitals)

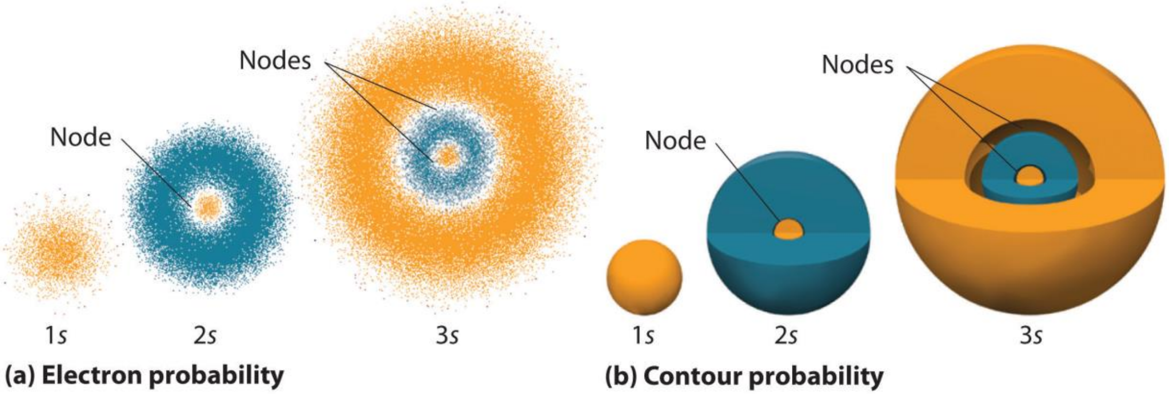
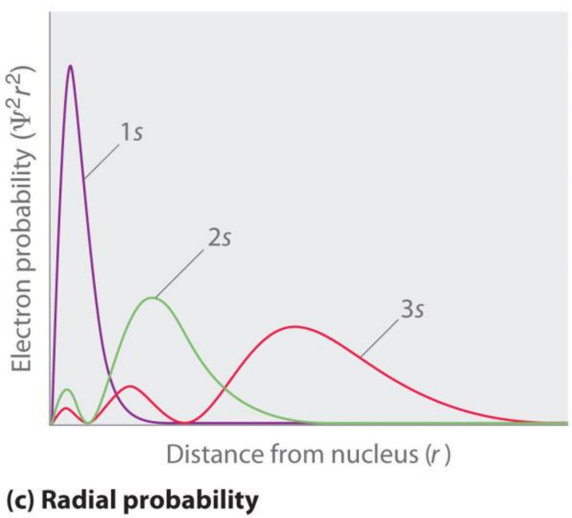


IMAGE COURTESY: [UCDAVIS CHEMWIKI](), [CC BY-NC-SA 3.0 US]()



1s orbital: 0 radial nodes
2s orbital: 1 radial node

What are nodes?

Regions where there is no probability of finding an electron

What is a radial node?

Depends on quantum numbers n and l

Radial node = n-1-*l*

Shapes of Atomic Orbitals; p orbital

How many p orbitals will there be in a shell?

Which is the first shell to have p orbitals?

What are nodes?

Regions where there is no probability of finding an electron

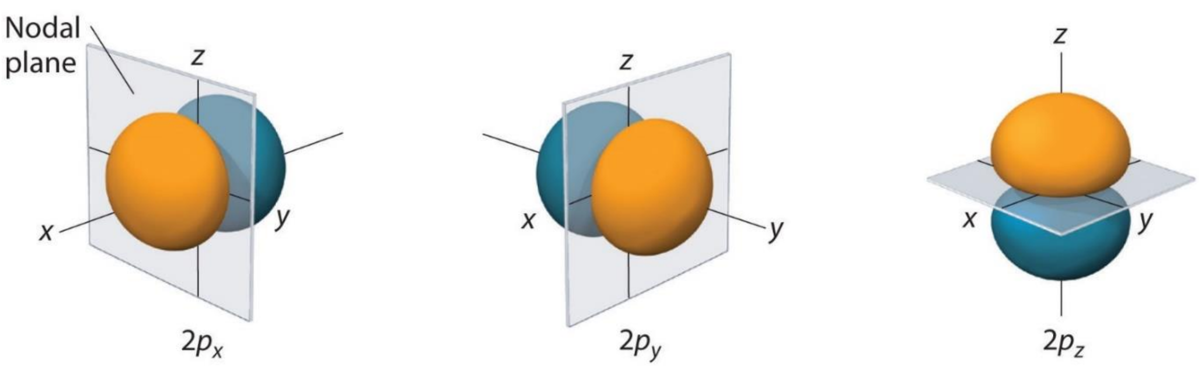


IMAGE COURTESY: [UCDAVIS CHEMWIKI](), [CC BY-NC-SA 3.0 US]()

What is an angular node?

Depends on quantum number *l*
Angular node = *l*

1s orbital: 0 angular nodes
2p orbital: 1 angular node

What does the radial distribution of a 2p orbital look like?

QUANTUM NUMBERS (describing orbitals)

1. Principal Quantum Number (n)

1. Positive integer (1,2,3….)
2. Indicates the relative size of the orbital – relative distance
3. Specifies the energy level (higher n indicated higher energy)

2. Angular Quantum Number (*l*)

1. Positive Integer (0 to n-1)
2. Shape of the orbital
3. The value of n limits *l*

if n=1, *l* can only have the value 0; if n=2, *l* can have the values 0 and 1

When l =0 (s orbital); l=1 (p orbital); l=2 (d orbital); l=3 (f orbital)

3. Magnetic Quantum Number (m_l)

1. Integer (-*l* to +*l*)
2. Orientation of the orbital around the nucleus
3. The value of l limits m_l; For l=1, values of m_l can be -1,0, and 1

Practice Problem 4 – Fill the table for n=1, 2, 3, and 4

n	l (0 to n-1)	m_l (-l to + l)	Subshell Designation	Number of orbitals in subshell	Number of orbitals in shell

Quantum Numbers

n	l (0 to n-1)	m_l (-l to + l)	Subshell Designation	Number of orbitals in subshell	Number of orbitals in shell
1	0	0			

l=0; s orbital   l=1; p orbital   l=2; d orbital   l=3; f orbital

Quantum Numbers

n	l (0 to n-1)	m_l (-l to + l)	Subshell Designation	Number of orbitals in subshell	Number of orbitals in shell
1	0	0	1s		

l=0; s orbital l=1; p orbital l=2; d orbital l=3; f orbital

Quantum Numbers

n	l (0 to n-1)	m_l (-l to + l)	Subshell Designation	Number of orbitals in subshell	Number of orbitals in shell
1	0	0	1s	1	1

l=0; s orbital   l=1; p orbital   l=2; d orbital   l=3; f orbital

Quantum Numbers

n	l (0 to n-1)	m_l (-l to + l)	Subshell Designation	Number of orbitals in subshell	Number of orbitals in shell
1	0	0	1s	1	1
2	0				
	1				

l=0; s orbital   l=1; p orbital   l=2; d orbital   l=3; f orbital

Quantum Numbers

n	l (0 to n-1)	m_l (-l to + l)	Subshell Designation	Number of orbitals in subshell	Number of orbitals in shell
1	0	0	1s	1	1
2	0	0			
	1	-1, 0, 1			

l=0; s orbital l=1; p orbital l=2; d orbital l=3; f orbital

Quantum Numbers

n	l (0 to n-1)	m_l (-l to + l)	Subshell Designation	Number of orbitals in subshell	Number of orbitals in shell
1	0	0	1s	1	1
2	0	0	2s		
	1	-1, 0, 1	2p		

l=0; s orbital   l=1; p orbital   l=2; d orbital   l=3; f orbital

Quantum Numbers

n	l (0 to n-1)	m_l (-l to + l)	Subshell Designation	Number of orbitals in subshell	Number of orbitals in shell
1	**0**	**0**	**1s**	**1**	**1**
2	**0**	**0**	**2s**	**1**	
	1	**-1, 0, 1**	**2p**	**3**	

l=0; s orbital   l=1; p orbital   l=2; d orbital   l=3; f orbital

Quantum Numbers

n	l (0 to n-1)	m_l (-l to + l)	Subshell Designation	Number of orbitals in subshell	Number of orbitals in shell
1	0	0	1s	1	1
2	0	0	2s	1	4 = 1 (2s) + 3 (2p)
	1	-1, 0, 1	2p	3	

l=0; s orbital l=1; p orbital l=2; d orbital l=3; f orbital

Quantum Numbers

n	l (0 to n-1)	m_l (-l to + l)	Subshell Designation	Number of orbitals in subshell	Number of orbitals in shell
1	**0**	**0**	**1s**	**1**	**1**
2	**0**	**0**	**2s**	**1**	**4 = 1 (2s) + 3 (2p)**
	1	**-1, 0, 1**	**2p**	**3**	
3	**0**	**0**	**3s**	**1**	**9 = 1(3s) + 3 (3p) + 5 (3d)**
	1	**-1, 0, 1**	**3p**	**3**	
	2	**-2, -1, 0, 1, 2**	**3d**	**5**	

l=0; s orbital   l=1; p orbital   l=2; d orbital   l=3; f orbital

Quantum Numbers

n (shell)	l (0 to n-1)	m_l (-l to + l)	Subshell Designation	Number of orbitals in subshell	Number of orbitals in shell
1	0	0	1s	1	1
2	0	0	2s	1	4 = 1 (2s) + 3 (2p)
	1	-1, 0, 1	2p	3	
3	0	0	3s	1	9 = 1(3s) + 3 (3p) + 5 (3d)
	1	-1, 0, 1	3p	3	
	2	-2, -1, 0, 1, 2	3d	5	
4	0	0	4s	1	16 = 1(4s) + 3 (4p) + 5 (4d) + 7 (4f)
	1	-1, 0, 1	4p	3	
	2	-2, -1, 0, 1, 2	4d	5	
	3	-3, -2, -1, 0, 1, 2, 3	4f	7	

Practice Problem 5: Quantum Numbers

Practice: Give the name, magnetic quantum numbers, and number of orbitals for each subshell with the given n and l quantum numbers:

(a) $n = 2, l = 1$

(b) $n = 1, l = 0$

(c) $n = 5, l = 2$

(d) $n = 3, l = 3$

Practice Problem 4: Quantum Numbers

Practice: Give the name, magnetic quantum numbers, and number of orbitals for each subshell with the given n and l quantum numbers:

(a) n = 2, l = 1 : 2p subshell; m_l = -1, 0, +1; 3 total orbitals

(b) n = 1, l = 0 : 1s subshell; m_l = 0 ; 1 total orbital

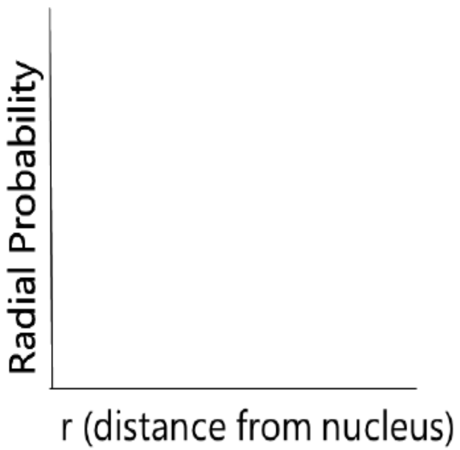
(c) n = 5, l = 2 : 5d subshell; m_l = -2, -1, 0, +1, +2 ; 5 total orbitals

(d) n = 3, l = 3: IMPOSSIBLE! (The highest value of *l* is n-1)

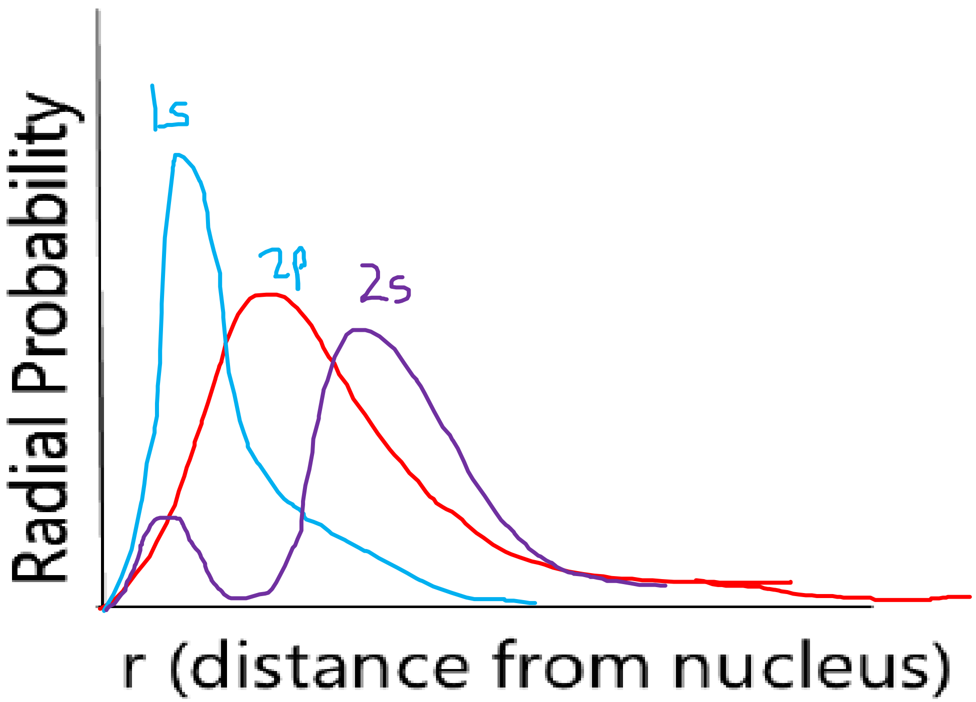
Practice Problem 6

Sketch the radial probability distribution for a 2p orbital

(For questions like these, you should be able to roughly determine the shape of the curve, keeping in mind the radial nodes. You are not expected to sketch a precise radial probability distribution chart.)

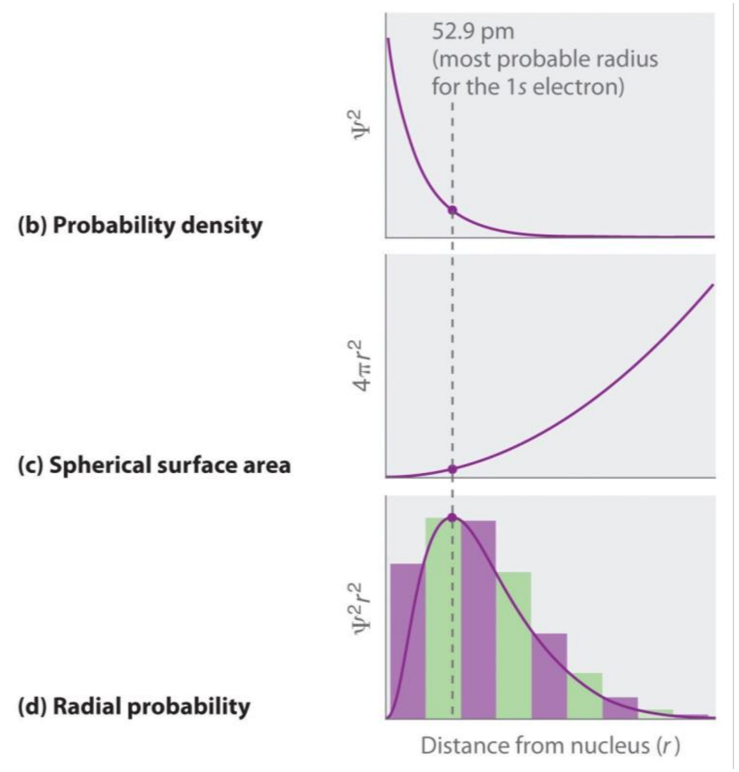


2p orbital – 0 radial nodes (n – 1 – l = 2 – 1 – 1 = 0)



Why did Bohr's Model work for hydrogen atom?

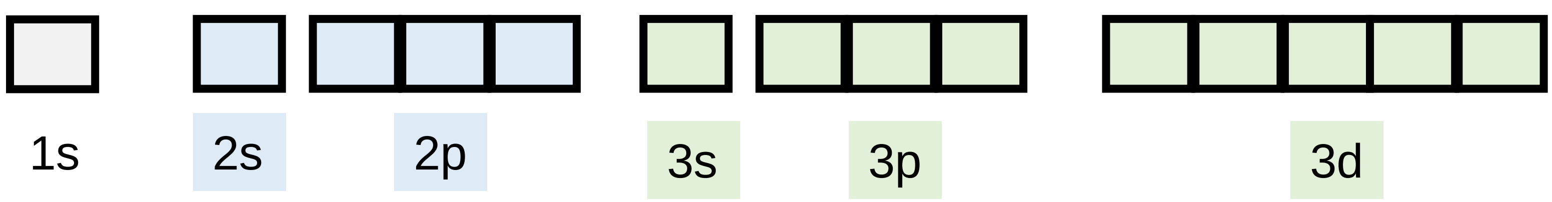
Bohr's model correctly predicted the radius of the H-atom – even though Bohr's atomic theory is incorrect. It cannot be applied to multi-electron species.
Why does it work for H?
Hydrogen is special – only one electron but there is more but there is more…..



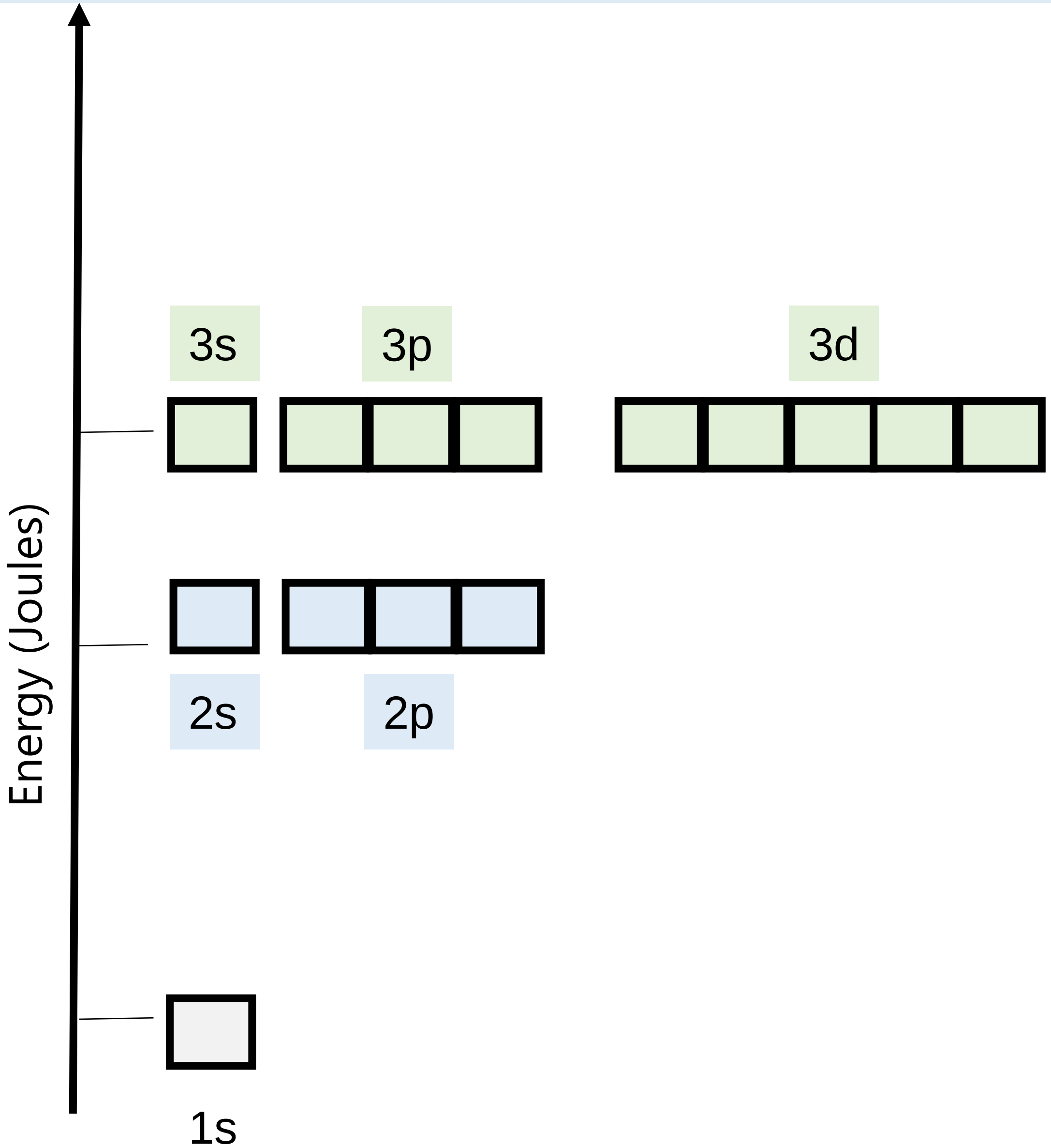
Why did Bohr's Model work for hydrogen atom?

Hydrogen is special – only one electron but there is more….

Can you draw the energy levels (energy of different orbitals based on increasing energy) for a H-atom?



Energy Levels of Hydrogen Atom



From Schrodinger Equation, we obtain the solution for the hydrogen atom

$$E_n = -\frac{m_e e^4}{8{\epsilon_0}^2 h^2 n^2}$$

slido

Which of these following transitions in a Hydrogen atom, will result in the highest amount of energy released? Explain your reason. (Assume all are allowed transitions)

ⓘ Start presenting to display the poll results on this slide.

Practice Problem 7

Which of these following transitions in a Hydrogen atom, will result in the highest amount of energy *released*? Explain your reason. (Assume all are allowed transitions)

A. From 1s to 2p
B. From 3p to 2s
C. From 5f to 2p
D. From 3p to 1s
E. From 1s to 5p
F. From 2p to 1s

We are looking for energy being released: So the transition must correspond to an electron going from a *higher n* to *lower n*

In hydrogen atom any transition to *n =1* will be higher in energy than a transition to any other *n* value.
The energy gap (for consecutive n values in hydrogen atom) between n=1 and n=2 is much larger as compared to that between n=2 and n=3, so on and so forth.