# Chem 001A Notes
# Week 4

Danny Topete

October 20th, 2025

# 1 Monday Lecture: Oct 20th

## 1.1 Emissions Spectra and the Bohr Model

- We are now struggling with the emission spectrum of atoms to solve that question

- Every atom or molecule has a discrete emission spectrum

- They are unique to each atom, treat them as a bar code

- Then Rydberg Equation developed a formula to predict the emission spectrum of atomic hydrogen:

$$\frac{1}{\lambda} = R(\frac{1}{n_1^2} - \frac{1}{n_2^2})$$

- Including Rydberg's constant to make it make sense

- Postulate Bohr model to figure out the spectrum model

1. Called hydrogen atoms to only allow certain energy levels, called **stationary states**.

2. Atom does not radiate energy while in a stationary state. (violation of classical physics)

3. Atom changes to another stationary state (another orbit) only by obsorbing or emitting a photon. Energy of photon (hv)...

- There is something about how atoms absorb photon to increase in energy level

- When they emit the photon, they decrease a level of energy (as observed in emission spectrum)

- Assuming this is actually happens, you can explain the emission spectrum, hence, why it is a postulate

- The energy level can be calculated as

$$E = const(\frac{1}{n_{final}^2} - \frac{1}{n_{init}^2})$$

- Looks a lot like Rydberg's equation

$$\Delta E = E_{final} - E_{init}$$

## 1.2 Limitations of Bohr Model

- Only predicts transition energyies for atoms

$$E = -2.18 \times 10^{-18} J \frac{Z}{n^2}$$

- This model requires quantum mechanics to fully understand the gaps

## 1.3 Quant descryption of hydrogen

- Going from Bohr model of "Orbits" $\rightarrow$ Quantum model of "Orbitals"

- F = ma = m $\frac{d^2x}{dt^2}$, "position function" x(t)

  This is a differential equation (I mean, both of them are). This is a time domain

- Wave Function, $\Psi$. H$\psi = E\psi$

  This is a frequency domain

- When it comes to these, there is an infinite number of solutions

- Orbitals can be identifies using combination of three integers called quantum numbers

- Ech orbital has a methamtically defined shape

- Each orbital has a probabilistic "location"(?)

- $n$ = Principle Quantum Number

  n = 1, 2,3, .., inf

- $L$ = Angular Momentum quantum number

  L = 0„1,2,...,n-1

- $m_I$ = Magnetic Quantum Number -l, -l, + 1, ..., 0, ..., l - 1, l

- Go to office hours to solve these differential equations

- When it comes for the # of orbitals, 2l + 1 = # of orbitals

- l = n-1, 0, -l, +l

## 1.4 Terms and definitions for QUant

- **Shell**: Given value of principle quantum number $n$. There are inf # of shells labelled $n = 1,2,..,$inf

- **Subshell:** each shell divided into subshells, determined by angular momentum quantum number $l$. For given shell with principle quantum number $n$, there are $n-1$ different subshells. Associated with each subshell is a letter designation.

| (n, l, m$_I$) | Orbital Name | # of orbitals |
|:---:|:---:|:---:|
| (2,0,m$_I$) | 2s | 1 |
| (2,1,m$_I$) | 2p | 3 |
| (4,2,m$_I$) | 4d | 5 |
| (4,3,1) | 4f | 1 |

Table 1: Orbital Information

- Electrons go down, orbitals are in a square

- Electrons have some mass, they have a charge

- Electrons also have a spin

- We had no idea where mass came from until a few years ago.

  Mass comes from the large hydron collider, and with sufficient energy. We get the Higgs field (Higgs boson). Particles interacting with the Higgs field makes mass.

- Spin exists, and use these properties to figure out how to put electrons into orbitals

# 2 Wednesday: Oct 22$^{th}$

## 2.1 Orbitals and electrons

- You can fit electrons in an orbital, this is within the probabilistic approach of where electrons would likely to be

- Electrons have a spin up (or a spin down; depending who you ask)

- Electron homes are called Shells

- Following derived from Shroder equation

$$H\Psi = (Energy)E\Psi(orbital)$$

- E $= \frac{1}{n^2}$, as n increases, so does energy

- One S-orbital 1, $1 = 1^2$

- One S-orbital and three P-orbitals $4 \rightarrow 1+3 = 2^2$

- 3x3 shell, one s-orbital, three p-orbitals, five d-orbitals, seven f-orbitals = 16

  $\rightarrow 1 + 3 + 5 + 7 = 4^2$

- Bohr's equation

$$E = (\frac{1}{n_f^2} - \frac{1}{n_i^2})$$

  There must be stationary states and we use that to define the energy states present. Until there is a transition between these states. As in, referring to shells (??)

  Used to describe the electron

- Quantum mechanics gives us the reason why Rydberg and Bohr models work out. They both bring in an integer, meanwhile Quantum helps solve for these constants

## 2.2 Shape of Hydrogen Orbitals

- Finish below later, something about the hydrogen orbital shape calculation

-
$$\psi_{n,l,m_I}(r,\theta,\phi) = NR_{n,l}(r)P_I$$

- P-orbitals, $p_z$, $p_x$ = m$_e$ = -1, $p_y$. Orientation is different based upon the cartesian coordinate system

- d-orbitals, look quite weird, flower shaped

- Should be able to identify the differences

- f-orbitals get even more intense, even weirdly shaped, more lobes

## 2.3 What does $\psi$ tell us

- This is all probabilistic

- Apple tree analogy

  - Map the apples fallen from an apple tree as a shell, then see the relationship of these apples
  - You will see most of them fall a bit away from the trunk, and less from the outside
  - Counting the number of apples within each circle
  - We get a distribution, a graph, in n apples per shell of trunk

  $$\psi^2 = probabilityDensity = \frac{probability}{unitVolume}$$

- Nodes are very specifically wave phenomnon, There are shells of very probability with wavelight behavior.

- As we go from 2s to 3s, we (s-1) roots where we hit zero, then end asymptotically zero

- p-orbitals → dumbbells

- d-orbitals → clover leafs

1. **Aufbau Principle:** Place electrons in the orbital with the lower possible energy

2. **Pauli Exclusion Principle:** Only one electron is allowed per quantum state i.e. two spin-paired electrons per orbitals

3. **Hund's Rule:** Place electrons in separate degenerate (same energy levels) orbitals before pairing

## 2.4 Putting electrons into orbitals

- Solutions are all approximated after Hydrogen