

# Chem 001A Notes

## Week 4

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### 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:

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

- 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 absorbing or emitting a photon. Energy of photon ( $h\nu$ )...
- 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

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

- Looks a lot like Rydberg's equation

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

## 1.2 Limitations of Bohr Model

- Only predicts transition energies for atoms

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

- This model requires quantum mechanics to fully understand the gaps

## 1.3 Quant description of hydrogen

- Going from Bohr model of "Orbits" → 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 identified using combination of three integers called quantum numbers
- Each orbital has a mathematically defined shape
- Each orbital has a probabilistic "location" (?)
- $n$  = Principle Quantum Number  
 $n = 1, 2, 3, \dots, \infty$
- $L$  = Angular Momentum quantum number  
 $L = 0, 1, 2, \dots, n-1$
- $m_L$  = Magnetic Quantum Number  $-l, -l+1, \dots, 0, \dots, l-1, l$
- Go to office hours to solve these differential equations
- When it comes for the # of orbitals,  $2l+1 = \#$  of orbitals
- $l = n-1, 0, -1, +1$

## 1.4 Terms and definitions for QUant

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

$(n, l, m_l)$	Orbital Name	# of orbitals
$(2, 0, m_l)$	2s	1
$(2, 1, m_l)$	2p	3
$(4, 2, m_l)$	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<sup>th</sup>

### 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
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$$\psi_{n,l,m_l}(r, \theta, \phi) = NR_{n,l}(r)P_l$$

- P-orbitals,  $p_z, p_x = m_l = -1, p_y$ . 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

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

- Nodes are very specifically wave phenomenon, There are shells of very probability with wavelength behavior.
  - As we go from 2s to 3s, we (s-1) roots where we hit zero, then end asymptotically zero
  - p-orbitals  $\rightarrow$  dumbbells
  - d-orbitals  $\rightarrow$  clover leaves
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

### 3 Friday lecture

#### 3.1 Back to electrons

- Previously we were looking at electron configurations
- This is a distribution function to where you are most likely to find these electrons, (then remember that there are some roots in the gaps; just like double slit wave behavior )
- The probability of where electron should be is like 98%
- As we go up in element, we keep populating the shells with electrons, until the next electron goes to the next electron
- Alkaline / alkaline metals were putting electrons into s-orbitals
- Going to the right of nonmetals, they put it into p-orbitals
- **Valence electrons**, electrons in the largest orbital, these are the ones that interact with the outside world. They are the ones to worry when bonding
- Core electrons are the ones within the inner shells
- Only exception we need to remember to half filled and full filled
  - Tungsten, W, Element #74, half filled shell
  - Group tells you how many electrons it has\*

#### 3.2 Periodic Trends

- Valence Electrons, occupying outer most shell (highest n) are called valence
- When talking of a charge of the outermost electron, the force. The outermost electron is not seeing a nucleus, rather one filled with electron shells. Those negative shells buffer the positive charge
- Calculate the nuclear charge, such as Li having two electrons in the s-orbital and 1 in the p-orbital, meaning it has a +1 charge ( $3(\text{proton}) - 2(\text{electrons in p-orbital})$ )