

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

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

- 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

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

- This model requires quantum mechanics to fully understand the gaps

1.3 Quant descryption 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, Ψ . $H\Psi = E\Psi$
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" (?)
- $n = \text{Principle Quantum Number}$
 $n = 1, 2, 3, \dots, \infty$
- $L = \text{Angular Momentum quantum number}$
 $L = 0, 1, 2, \dots, n-1$
- $m_L = \text{Magnetic Quantum Number}$ $-l, -l+1, \dots, 0, \dots, l-1, l$
- Go to office hours to solve these differential equations
- When it comes for the # of orbitals, $2l + 1 = \# \text{ of orbitals}$
- $l = n-1, 0, -l, +l$

1.4 Terms and definitions for QUant

- **Shell:** Given value of principle quantum number n . There are inf # of shells labelled $n = 1, 2, \dots, \text{inf}$
- **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_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 22th

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

$$H\Psi = (\text{Energy})E\Psi(\text{orbital})$$

- $E = \frac{1}{n^2}$, 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

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

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
- $\psi_{n,l,m_I}(r, \theta, \phi) = N R_{n,l}(r) P_I$
- 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 ψ 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 wavelight 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 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

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 elcton 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 outmost electron is not seeing a nucleus, rather one filled with electron shells. Those negative shells bugger 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 ($3(\text{proton}) - 2(\text{electrons in p-orbital})$)